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Propagation of supersonic soliton in carbon nanotubes of armchair type

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The propagation of a localized ring nonlinear wave in carbon nanotubes (CNTs) of armchair type has been explored using the MD/DFTB method. It is unambiguously shown that the considered localized waves are soliton-type. Herewith, the higher a velocity of an initial perturbation, the higher a steady-state velocity of the considered soliton. It is established that at a high initial excitation energy in a time period of 0.1−0.2 ps the soliton moves at the speed in the range of 245−270 Å/ps, which is approximately in 1.22−1.35 times higher than the speed of sound in CNTs (200 Å/ps). It is shown that the soliton velocity practically does not change with increasing CNT radius

Keywords: molecular dynamics, carbon nanotubes, soliton, supersonic wave.

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Introduction

In two-dimensional atomic lattices, high energy perturbations propagate as localized waves (solitons, breathers, crowdions, etc.) [1,2]. If the lattice elements are distributed equidistantly along the wave propagation axis, as, e.g., in a triangular lattice, then the wave moves in a natural way [3–6]. However, in lattices whose atoms are distributed unevenly, as, e.g., in graphene, energy is dissipated faster into unperturbed rows, and waves decay faster [7,8]. Nonlinear waves were considered in a recent work in another two-dimensional material — phosphorene [9]. Unexplored is the propagation of ring waves in carbon nanotubes (CNTs), in which the initial perturbation is applied to all end atoms. Earlier the authors considered the propagation of a soliton-like ring wave arising due to pulse excitation of longitudinal speed at each end atom of the zigzag end of a perpendicularly trimmed tube [10]. The object of this study is CNTs of the „zigzag“ type with chiralities (8,8), (9,9), (10,10). In this case, one of the important tasks of the study is to show that the excited ring wave in such tubes is a supersonic soliton.

1. Method of study

The main research method was the classical method of molecular dynamics with the integration time step $dt = 0.1$ fs. The force acting on the atom at each step was calculated within the density functional theory based on the Self-Consistent Charge Density Functional Tight-Binding (SCC DFTB) method [11]. The total energy within the framework of this method can be found as the sum of the band structure energy E_{BS}, the repulsive energy E_{rep}, and the energy that takes into account charge transfer on atoms E_{SCC}:

$$E_{\text{tot}} = E_{BS} + E_{\text{rep}} + E_{SCC}. \quad (1)$$

The equilibrium position of the structures under study was found by minimizing the expression (1) by changing the coordinates of the atoms until the maximum force acting on the atom did not exceed 10^{-5} eV/Å. The basis set pbc-0-3 [12] was used to describe the interaction of carbon atoms. The use of the SCC DFTB method allows taking into account quantum effects, which are often neglected in molecular dynamics studies of low-dimensional structures, while the method itself is less energy-consuming compared to the DFT method. In this regard, the DFTB potential is often used in molecular dynamics modeling of low-dimensional structures [13,14].

2. Results

Let us consider an atomistic model of CNT (9,9) with a length of 120 Å (Fig. 1). Let us impart the initial velocity equal to 80 Å/ps to each end atom of the chair-shaped end along the tube axis and start the molecular dynamics with a length of 0.3 ps.

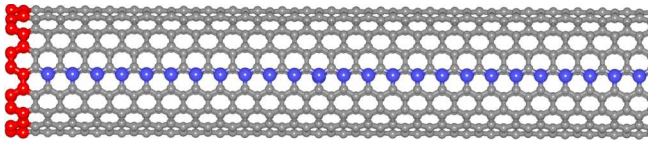

Figure 1. A fragment of the atomistic model of the investigated CNT (9,9). The ring wave is excited due to the initial momenta received by the end atoms (highlighted in red in the online version) directed along the tube axis. The velocities of atoms at each moment of time are fixed in a row of atoms marked with blue circles (in the online version).

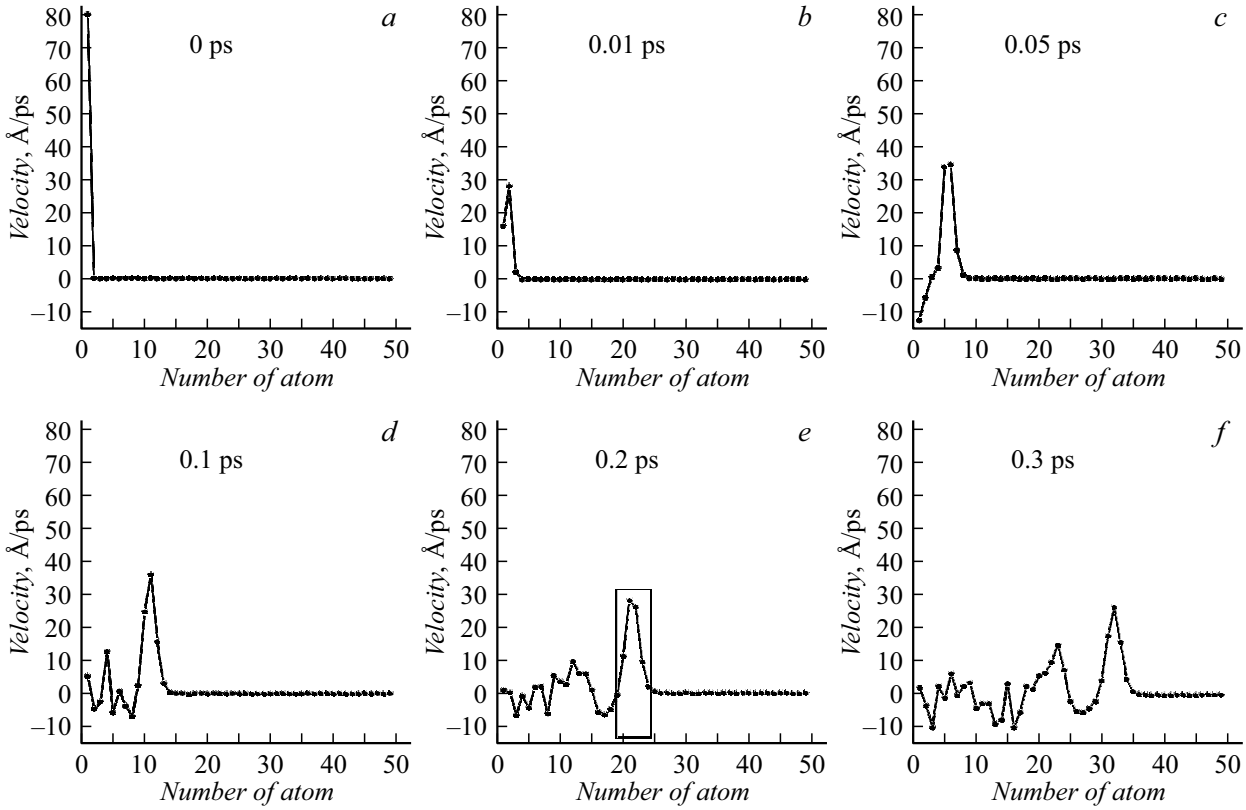

Figure 2. The distribution of the longitudinal velocity of atoms v_i in one longitudinal row of a nanotube at different times, the initial velocity of atoms being $v_0 = 80$ Å/ps.

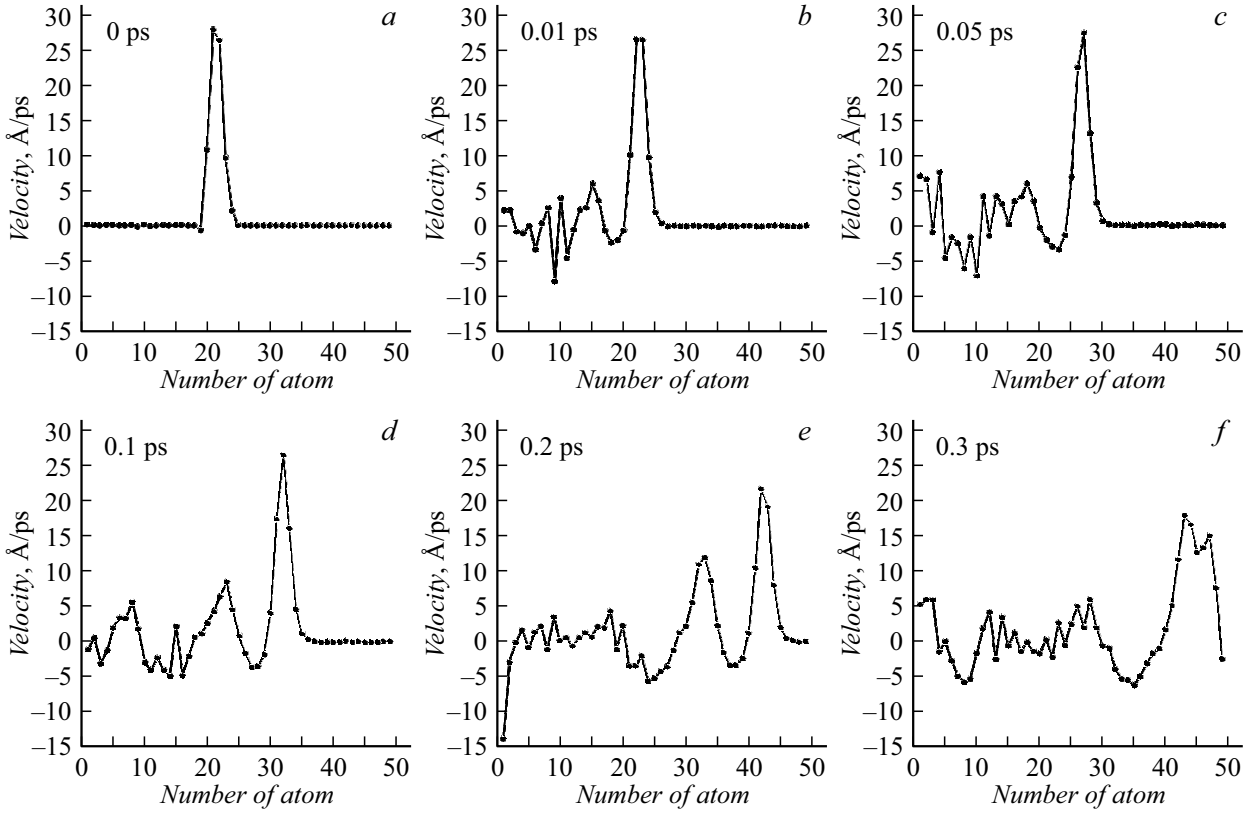

Figure 3. The distribution of the longitudinal velocity of atoms v_i in one longitudinal row of a nanotube depending on time.

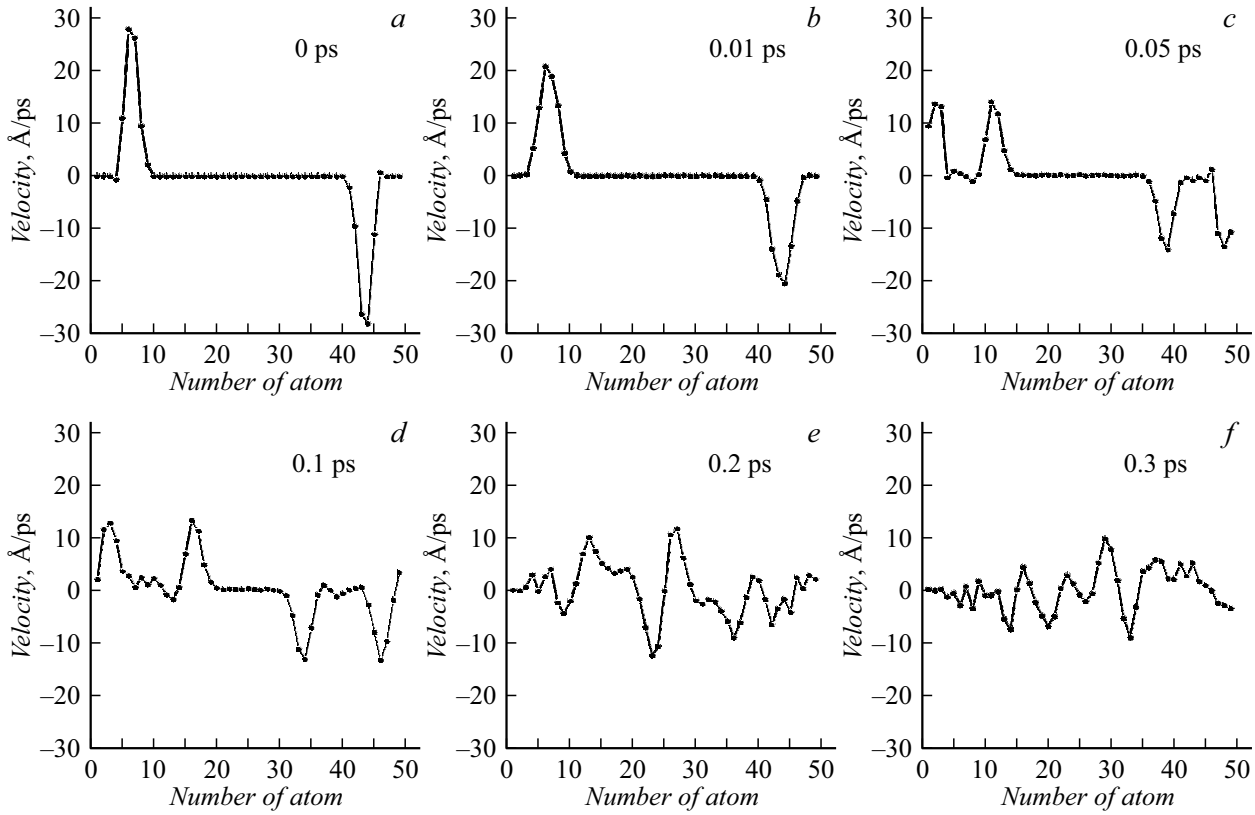

Figure 4. Plots of changes in the propagation velocity of two symmetrical counterpropagating solitons. The symmetry of the atomic velocity distribution is preserved throughout the time, even after the collision of solitons.

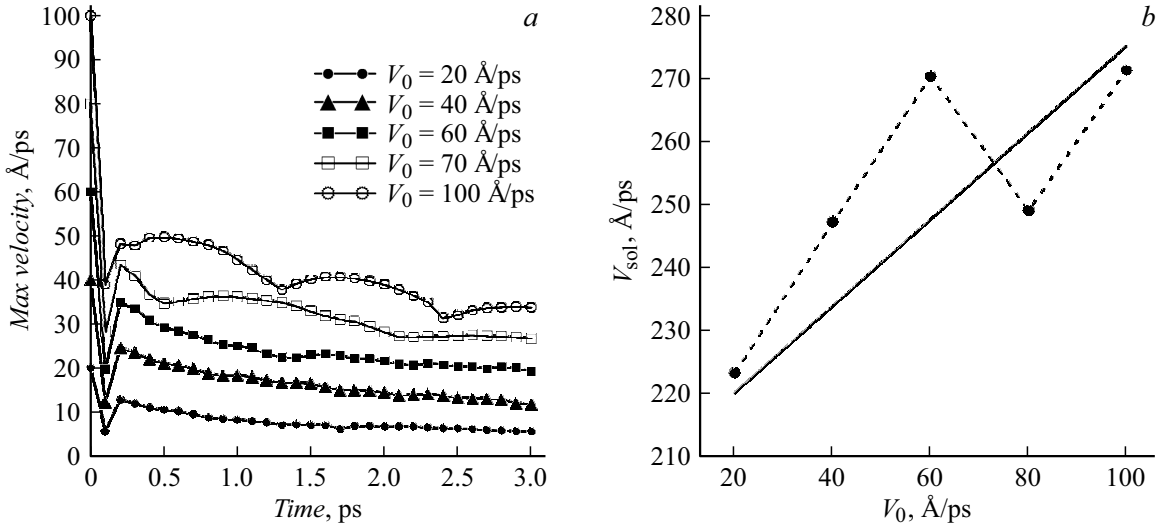

Figure 5. *a* — temporal evolution of the maximum velocity of atoms in a CNT; *b* — dependence of the ring soliton velocity in a nanotube on the velocity of particles in the end layer at the initial moment of time. Dots show the velocities calculated for the time interval 0.1–0.2 ps, the dashed line shows the dependence of the soliton velocity at different values of the initial velocity, the solid line is the approximating line.

The distribution of the longitudinal velocity of atoms v_i in one longitudinal row of a nanotube at different times is shown in Fig. 2. It can be seen that already after 0.05 ps, a velocity peak ($v_{max} \approx 30$ Å/ps) is formed, which persists with further wave propagation. It follows from Fig. 2 that the excited localized wave can be classified as a supersonic soliton, since no other perturbations are observed ahead of it.

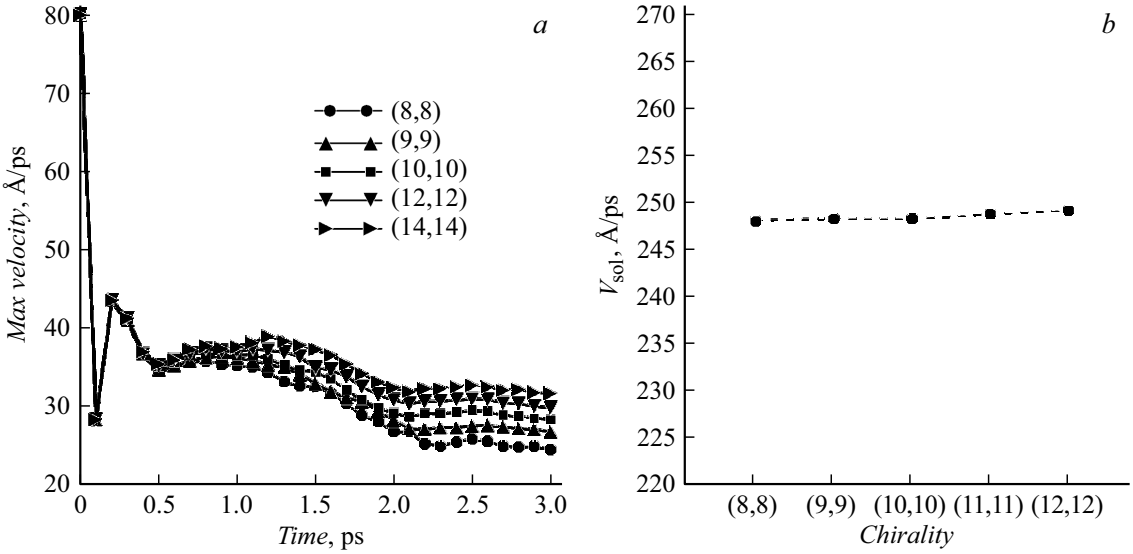

Figure 6. *a* — temporal evolution of the maximum velocity of atoms in a CNTs with different diameters (the initial velocity is $v_0 = 80$ Å/ps); *b* — dependence of the ring soliton velocity in a nanotube on the nanotube radius. Dots show the velocity values calculated for the time interval 0.1−0.2 ps, the dashed line shows the dependence of the soliton velocity at different values of the radius.

To test this hypothesis, we use the state $v_0 = 80$ Å/ps, $t = 0.2$ ps as a sample for setting the initial conditions. In Fig. 3, *e* the velocity maximum is observed at $n = 21$, for $n < 19$ and $n > 24$ the velocity is assumed to be zero, and the deviations of the coordinates from the equilibrium values are considered equal, like those of $n = 19$. The soliton is formed by compression of the tube to the left of the soliton, and the tube to the left of the soliton is in equilibrium, but all particles are shifted from their equilibrium positions to form compression in the region of the soliton.

Having started molecular dynamics from the state of the system shown in Fig. 3, *a*, we trace the changes in the soliton propagation velocity versus the atom number in the row. It can be seen that the lattice perturbations to the left of the soliton are small, and the dip located directly behind the main peak can be considered part of the soliton (Fig. 3).

Consider the meeting of two similar solitons launched from opposite ends of the tube. For the second soliton, we take a mirror-reflected excitation directed from right to left. Calculations will be carried out during the same time. The plots obtained (Fig. 4), first, undoubtedly confirm that the localized waves under consideration are of the soliton type. They pass through each other at a meeting, practically without changing. Therefore, the initial soliton can be used without fear that a high-power tail will immediately form behind it. Second, it is very important that the detected soliton includes perturbations of the transverse velocity and coordinate components. The surface of the tube becomes slightly „corrugated".

Let us now estimate the dependence of the velocity of a ring soliton in a nanotube on the velocity of particles in the end layer at the initial moment of time. For this purpose, we will carry out experiments where the initial velocity at the end atoms of CNT (9.9) is equal to 20, 40, 60, and 100 Å/ps.

Let us consider the dependence of the maximum velocity of particles in a nanotube on time for different initial velocities of particles in the end layer. It can be seen from Fig. 5, *a* that the length of the transient process is approximately 0.025 ps, which follows from the time dependence of the maximum particle velocity over the ensemble. By this time, the maximum values of particle velocities are established, which are approximately two times lower than the initial velocities and which then remain almost unchanged during the rest time of the study. It is seen that the higher the initial perturbation velocity, the higher the steady state velocity of the soliton under study. Let us consider the dependence of the velocity of a ring soliton in a nanotube on the velocity of particles in the end layer at the initial moment of time. The soliton velocity was estimated from the average distance traveled by the soliton during the time interval 0.1−0.2 ps, the soliton coordinate being associated with the maximum in the velocity distribution. Since this distribution is a discrete function, the accuracy of velocity determination was not very high, as the distance traveled in 0.1 ps was not more than 26.8 Å, while the sampling step was one hexagon. From Fig. 5, *b* we can conclude that with an increase in the energy of the initial excitation, the soliton velocity increases to values of 245 and 270 Å/ps, which is approximately 1.22−1.35 times greater than the velocity of sound in CNTs (200 Å/ps).

Let us now estimate the dependence of the velocity of a ring soliton in a nanotube on the value of the CNT radius. To do this, we will carry out experiments with CNTs (8.8), (9.9) and (10.10). Let us take the initial velocity of the end atoms equal to 80 Å/ps. Consider the

maximum velocity of particles in a nanotube at different CNT radii (Fig. 6, *a*). The length of the transient process in this Figure is also approximately equal to 0.025 ps, by this time the maximum value of the particle velocity establishes, which then remains almost unchanged during the rest of the study time. Obviously, the velocity of the studied soliton is practically independent of the CNT radius. Only after 0.2 ps one can notice that the smaller the CNT radius, the lower the soliton velocity, but these effects are minor. Let us also plot the dependence of the velocity of a ring soliton in a nanotube on the CNT radius, which is controlled by the chirality indices (Fig. 6, *b*). The soliton velocity was estimated from the average distance traveled by the soliton during the time interval 0.1−0.2 ps, the soliton coordinate being associated with the maximum in the velocity distribution. It is shown that the soliton velocity practically does not change with increasing CNT radius (the velocity change does not exceed 0.4 Å/ps). On the whole, it can be assumed that there is no relationship between the velocity of a ring soliton in a nanotube and the CNT radius. This issue requires a separate consideration for a more accurate determination of this dependence — it is necessary to consider tubes with other radii, as well as to consider processes with other initial velocities of end atoms.

Conclusion

With the help of the molecular dynamics method based on the SCC DFTB potential, it is unambiguously shown that in „armchair“ type CNTs, the propagation of soliton-type waves obtained by excitation of atoms at the end is possible. Both the propagation of one localized nonlinear wave and the interaction of two counterpropagating waves excited at different ends of a tube of finite length 120 Åare considered. It is shown that the wave propagation velocity increases with the energy of the initial perturbation, and when localized waves meet, they pass through each other practically without distortion, which proves the soliton nature of the wave processes under study. It is found that at a high initial excitation energy in the time period 0.1−0.2 ps, the soliton moves with a velocity in the range 245−270 Å/ps, which is about 1.22−1.35 times higher than the speed of sound in CNTs (200 Å/ps). It is shown that the soliton velocity insignificantly grows with increasing CNT radius.

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Conflict of interest

The authors declare that they have no conflict of interest.

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