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Dynamics of a localized ring nonlinear wave in a carbon nanotube

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The propagation of nonlinear localized soliton-like super-acoustic longitudinal waves in a carbon nanotube was explored by the molecular dynamics modeling. Ring waves were excited by pulsed action on all the atoms of the edge zigzag layer and they got an initial velocity along the axis of the nanotube. It was shown that the velocity of a localized (soliton-like) ring super-acoustic wave increased with an increase in the initial velocity of the edge atoms. The calculated dependence of the propagating wave velocity on the initial velocity of the edge atoms was given.

Keywords: carbon nanotube, ring nonlinear waves, molecular dynamics.

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As a rule, high energy perturbations propagate across two-dimensional lattice molecular structures in the form of localized waves (solitons, breathers, kinks, crowdions, etc.) [1]. The reason for such dynamics is the competition of nonlinear and dispersive properties of the lattices, the former associated with nonlinearity of the coupling potentials of lattice elements, while the latter are due to discreteness of lattice structures. Wave propagation along some crystallographic axis occurs naturally if the lattice elements are distributed equidistantly along that axis, as, for example, in the triangular lattice [2–5]. In that case, the wave can propagate either down a single row of the lattice or M adjacent rows [3]. However, the wave has a limited lifetime, because part of the energy is spent on perturbing oscillations in the adjacent rows. The lifetime and trajectory length of the wave before its dissipation increase with the number M of the initially excited rows, since the energy is lost mainly into the running perturbations in the outer series, associated with the first unperturbed part of the lattice. For example, in a triangular lattice with Morse potential, this dependence is almost linear [5]. But energy dissipation into the unperturbed rows occurs much faster in lattices in which there are no directions along which the atoms would be evenly spaced, as, for example, in the hexagonal lattice of graphene (see, for example, study [6] and the extensive bibliography given there). However, the effect of energy pumping into the initially unperturbed rows is not naturally realized in case the two-dimensional lattice is rolled into a tube, and the initial speed perturbation along the tube axis is applied to all end atoms, resulting in a ring wave propagating through the tube.

The target of the present study is a carbon nanotube (16,0), since that type of tube is the one most frequently synthesized among the achiral tubes [7]. We consider the dynamics of propagation of a localized soliton-like ring wave arising during pulse excitation of longitudinal speed at each end atom of the zigzag end of a perpendicularly trimmed tube. The wave runs along the „chair“direction, and excitations in each longitudinal row of atoms are identical, which is ensured by the achirality of the tube. The main purpose of the study is to determine the speed of the soliton-like wave as a function of the initial momentum (initial speed) received by the end atoms.

The evolution of displacement and speed of each tube atom is investigated in a molecular dynamic study based on the strong coupling method in the SCC DFTB (self-consistent charge density functional tight-binding) theory approximation [8], according to which the total energy of the system is determined by the expression

$$E_{tot} = E_{\mathrm{BS}} + E_{rep} + E_{\mathrm{SCC}}, \qquad (1)$$

where E_{BS} is the energy of the band structure, E_{rep} is repulsion energy, E_{SCC} is the correction for self-consistency of atom charges. In particular, this method enables accounting for the shift of the electron cloud of every atom, which makes the numerical experiment as close to the real one as possible. Previously, the SCC DFTB method has been successfully applied to simulate the growth of carbon nanotubes [9] and analyze their mechanical and electronic properties [10]. Fig. 1 shows atom speed distributions in one of the tube rows oriented along its axis at sequential time moments following a small initial pulse (upper fragments) and a significant impact (lower fragments).

It follows from the figures presented that the localized disturbance propagating along the tube can be classified as a supersonic soliton-like wave, since it is weakly deformed in motion and is supersonic, no disturbances observed ahead of it. However, in these experiments dynamic perturbations of the tube structure after the passage of the initial pulse are quite strong. This is due to the fact that the initial form of perturbation in the tube, caused by an external pulse, does not fully correspond to the soliton structure. A powerful pulse is only released after some transient process, which

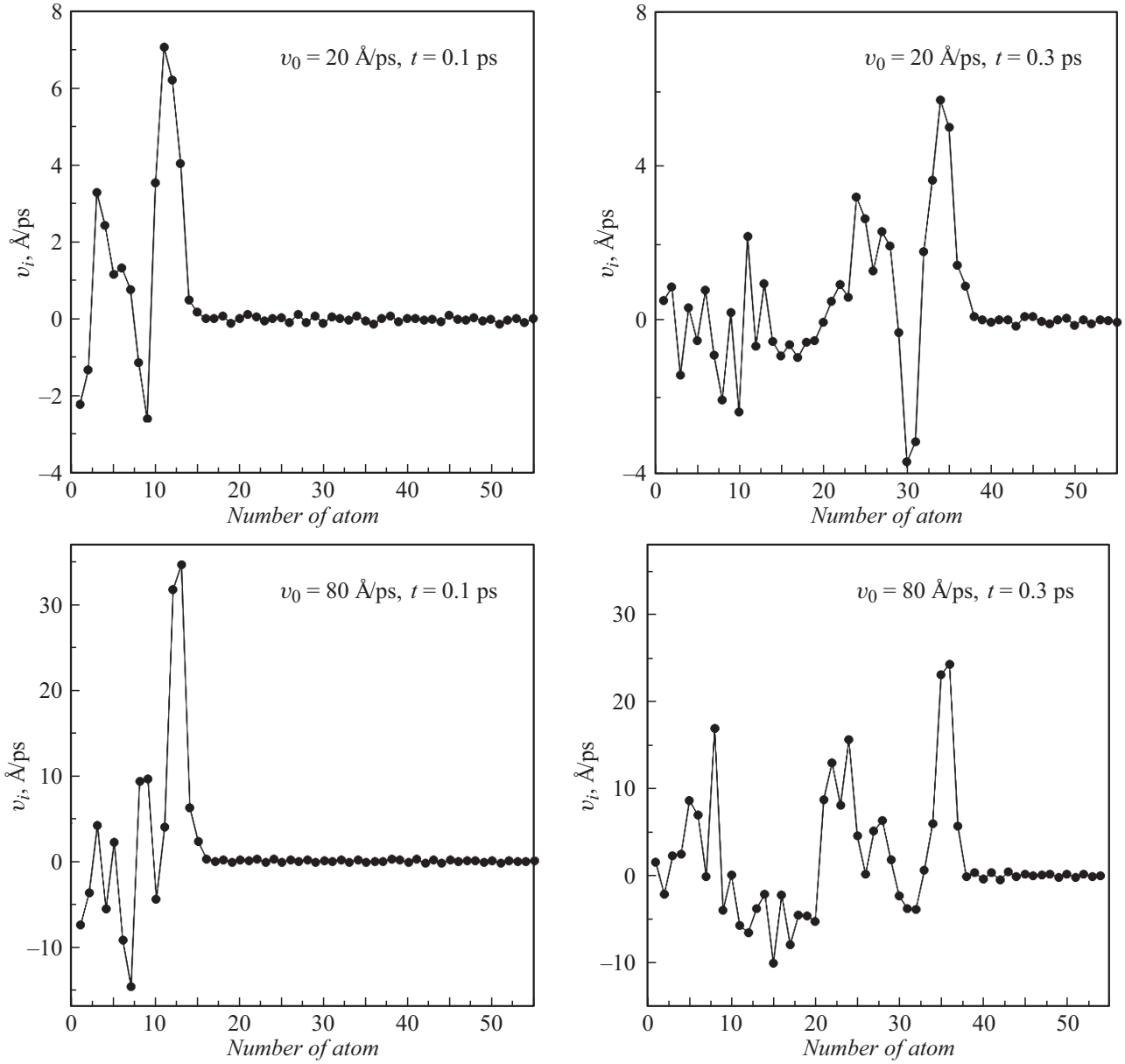

Figure 1. Distribution of longitudinal speed of atoms v_i in one longitudinal row of a nanotube at consecutive time points $t = 0.1$ and 0.3 ps at small ($v_0 = 20$ Å/ps) and high ($v_0 = 80$ Å/ps) initial speed of the end atoms.

runs at a speed above the speed of sound and is estimated in this case to be close to 200−220 Å/ps. Duration of the transition process is approximately 0.1 ps, which follows from the time dependence of the maximum ensemble speed of the particles (Fig. 2). It can be seen that the maximum particle speed is established by that time and suffers almost no changes for at least 0.2 ps. Note that the length of the simulated nanotube was small: 55 hexagons (119.7 Å). The steady-state maximum particle speed in the generated running pulse is about 3 times less than the initial value v_0 in the range from 10 to 120 Å/ps.

All of these speed values are significantly lower than the speed of sound and, moreover, the speed of a soliton-like wave retrieved from the results of the computer experiment. That speed was estimated from the average distance traveled by the soliton over the time interval 0.1−0.2 ps, the coordinate of the „soliton“ associated with the maximum in the particle speed distribution (Fig. 2). Since that distribution is a discrete function, the accuracy of speed determination was not very high, as the distance traveled in 0.1 ps was not more than 28.4 Å, while the sampling step was one hex. Nevertheless, it is shown unambiguously that the soliton-like wave speed increases with the initial speed of the end-layer particles (Fig. 3). At moderate v_0 the speed of the soliton wave grows almost proportional to v_0, but when it approaches the limit value for the nanotube, not resulting in the tube deformation yet, the dependence $v_{sol}(v_0)$ tends to saturate at $\sim (1.4-1.5)$ the speed of sound (assuming

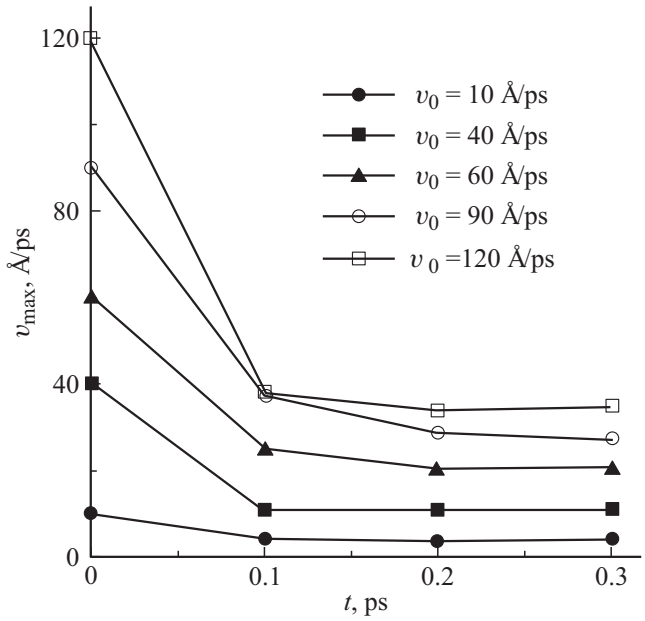

Figure 2. Evolution of the maximum particle speeds in a nanotube for different initial particle speeds of the end layer. It can be seen that by the time $t = 0.1$ ps the maximum speed reaches an almost constant level, which indicates the completion of soliton formation. The soliton propagates at an almost constant speed.

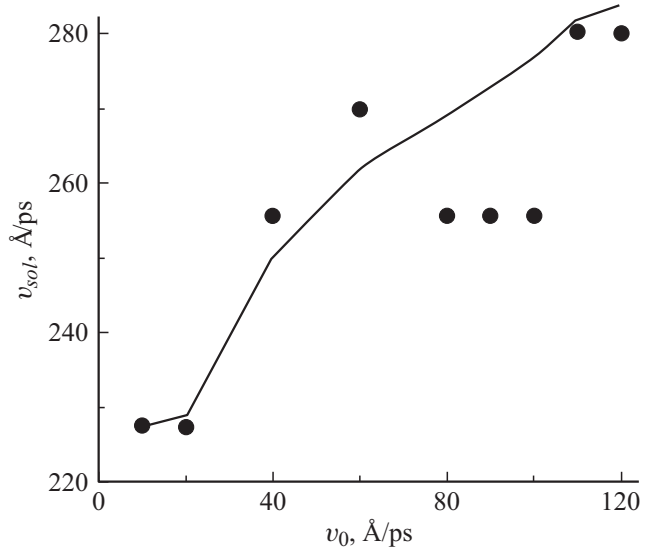

Figure 3. Ring soliton speed in a nanotube vs. the speed of the end-layer particles at the initial moment of time. Dots show the speeds calculated for the time interval 0.1−0.2 ps, the solid line shows the averaged dependence of soliton speed for different initial speeds.

the speed of sound in the carbon nanotube is ~ 200 Å/ps under the experiment conditions). Since the initial excitation energy increases in proportion to v_0^2, we can conclude that this increase in wave speed by about 40−50% occurs when the initial energy increases more than 100-fold.

Apparently the atoms of the tube move not only along its surface, but across it as well during wave propagation, which also consumes wave energy. However, that issue requires separate consideration. Also one of the possible directions of further research is to consider soliton-like waves in non-carbon nanotubes [11].

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Conflict of interest

The authors declare that they have no conflict of interest.

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