INTRODUCTION

In the past few decades, increased attention from researchers has been attracted to localized excitations of the soliton type. Their role in various relaxation and deformation processes is pronounced quite clearly [1–5]. The concept of static topological solitons is useful in studying an imperfect crystal structure [6, 7] and their mobility is responsible for the specific “soliton” contribution to the thermodynamics and kinetics of a polymer crystal.

However, theoretical analysis of soliton excitations with consideration of the actual structure of macromolecules forming a crystal presents substantial difficulties related to the nonlinear character of the equations of soliton dynamics and the multicomponent nature of the system. For this reason, schematic models of polymer chains are usually considered, which permit reduction to a one-component system. Application of a numerical–variational method of finding soliton solutions [10, 11] made it possible to successfully overcome the aforementioned difficulties in the case of an isolated chain [8, 9]. This method was used to study topological solitons in crystalline polyethylene (PE) [12–14]. Within the framework of a realistic model taking account of deformations of valence bonds, bond angles, and torsion angles, as well as intermolecular interaction of neighboring chains, three types of topological solitons describing local topological defects in a PE crystal were revealed. These solitons correspond to the extension or contraction of a chain zigzag by the lattice spacing, the extension or contraction by half lattice spacing with a simultaneous twist by 180°, and a pure twist of a zigzag by 360°.

By now, PE has been most extensively studied as belonging to the class of macromolecules with a repeating unit consisting of a single carbon atom. The ground state of this molecule is a flat zigzag chain conformation (or a helix denoted as 1 ∗ 2/1). The two-dimensional character of this zigzag chain accounts for certain significant features of its dynamics. However, for most macromolecules of this kind, the preferred conformation is that of a three-dimensional helix rather than a planar zigzag. So, it is of interest to study topological solitons in a crystalline polymer with macromolecules taking a three-dimensional helix conformation in the ground state. Poly(tetrafluoroethylene) (PTFE) is the simplest example of such a polymer.

PTFE molecules are PE analogs. The ground state of a PTFE molecule is a three-dimensional helix denoted as 1 ∗ 13/6. The studies of the nonlinear dynamics of an isolated PTFE molecule revealed that the helical shape of the chain gives rise to the existence of a new type of acoustic solitons—the solitonic torsional wave—in this macromolecule [15, 16]. The aim of this work is to study the dynamics of topological solitons in a helical polymer macromolecule using PTFE as an example. We will show that four types of topological defects exist in a helical macromolecule, with one of them exhibiting the soliton dynamics.

MODEL

At temperature $T < 19^\circ C$, a PTFE molecule in a crystal has the form of a 13/6 helix, i.e., there are 13 CF$_2$ groups per 6 revolutions of the helix. The lattice constants are $a = b = 5.59$ Å, $c = 16.88$ Å [17]. The
angle of the helix is \( \Delta \phi = 12 \pi / 13 = 166.15^\circ \), and the pitch is \( \Delta z = c/13 = 1.298 \ \text{Å} \).

The helix radii about carbon atoms \( \rho_c \) and fluorine atoms \( \rho_f \) can be determined from the values of the CC and CF bond lengths and the FCF bond angle:

\[
\rho_c = \left[ \left( \rho_{cc}^2 - \Delta z^2 \right) / 2(1 - \cos \Delta \phi) \right]^{1/2},
\]

\[
\rho_f = \left[ \rho_f^2 + 2 \rho_c \rho_{cf} \cos (\alpha_{fcf}/2) + \rho_{cf}^2 \right]^{1/2}. \tag{2}
\]

According to [18], the bond lengths are \( \rho_{cc} = 1.54 \ \text{Å} \) and \( \rho_{cf} = 1.34 \ \text{Å} \) and the bond angle is \( \alpha_{fcf} = 104.8^\circ \). Thus, from Eqs. (1) and (2) we obtain \( \rho_c = 0.417 \ \text{Å} \) and \( \rho_f = 1.628 \ \text{Å} \).

In the equilibrium state, the position vector of the \( n \)th carbon atom \( C_n \) is

\[
R_{c_n} = (\rho_c \cos (n \Delta \phi), \rho_c \sin (n \Delta \phi), n \Delta z),
\]

and the position vectors of the first and second \( n \)th fluorine atoms \( F_{n}^\pm \) are

\[
R_{f_n^\pm} = (\rho_f \cos (n \Delta \phi \pm \beta), \rho_f \sin (n \Delta \phi \pm \beta), n \Delta z),
\]

where \( \beta = \arcsin (\rho_{cf} \sin (\alpha_{fcf}/2)/\rho_f) = 40.69^\circ \). Thus, a PTFE molecule is described as three left-handed helices (one going through \( C_n \) atoms and two, through \( F_{n}^\pm \) atoms).

In a crystal, each macromolecule is surrounded by six neighbor molecules (Fig. 1). Let us consider interaction of these chains. The nearest four molecular chains are right helices with the position vectors

\[
R_{c_n} = \left( \pm \frac{a'}{2} + \rho_c \cos (\phi_0 - n \Delta \phi), \right.
\]

\[
\left. \pm \frac{b'}{2} + \rho_c \sin (\phi_0 - n \Delta \phi), \right)
\]

\[
\left. z_0 + n \Delta z \right),
\]

\[
R_{f_n^\pm} = \left( \pm \frac{a'}{2} + \rho_f \cos (\phi_0 - n \Delta \phi \pm \beta), \right.
\]

\[
\left. \pm \frac{b'}{2} + \rho_f \sin (\phi_0 - n \Delta \phi \pm \beta), \right)
\]

\[
\left. z_0 + n \Delta z \right),
\]

where \( \phi_0 \) and \( z_0 \) are the relative angular and longitudinal advances of the helices. The two other nearest helices are obtained from the initial one by shift along the \( Y \)-axis by \( \pm b' \).

We can calculate the unit cell parameters of a PTFE crystal by minimizing the energy of nonvalence interaction of helices with respect to the four parameters \( a', b', \phi_0, \) and \( z_0 \). Describing the interaction of atoms belonging to neighbor chains (CC, CF, and FF) by the pair potentials proposed in [18], we obtain \( a' = 9.41 \ \text{Å}, b' = 5.72 \ \text{Å}, \phi_0 = -110.77^\circ, \) and \( z_0 = 1.95 \ \text{Å} \). Figure 1 presents the relative arrangement of the helices. Further in the simulation of the dynamics of a molecular chain, the six nearest neighbor chains will be assumed to be immobile. These chains comprise an immobile substrate for the molecular chain under consideration.

Let us use the approximation of united atoms and consider the repeat unit \( CF_2 \) of a PTFE macromolecule as a single particle of mass \( M = 50m_p \) (where \( m_p \) is the
where \( R = (R_0 \cos(n \Delta \phi), R_0 \sin(n \Delta \phi), n \Delta z) \), where \( R_0 = \rho_c \) is the helix radius.

The equilibrium value of the \( \angle \text{CCC} \) bond angle is 
\[
\theta_0 = \arccos\left\{ \frac{-\langle e_{n-1}, e_n \rangle}{\rho_0^2} \right\},
\]
where \( e_n = R_{n+1} - R_n \) is the vector determining the direction of the nth bond and \( \rho_0 = \rho_{\text{CC}} \) is the equilibrium bond length. After elementary transformations, we obtain
\[
\theta_0 = \pi - \arccos\left\{ \left[ 4R_0^2 \sin^2(\Delta \phi/2) \cos \Delta \phi + \Delta z^2 \right] / \rho_0^2 \right\} = 116.30^\circ
\]

The equilibrium value of the nth dihedral (torsion) angle is
\[
\eta_n = \arccos\left\{ \left( \mathbf{v}_{n-1}, \mathbf{v}_n \right) / |\mathbf{v}_{n-1}| |\mathbf{v}_n| \right\}
\]
\[
\eta_0 = \arccos\left\{ \left( h^2 \cos \Delta \phi + \sin^2 \Delta \phi \right) / h^2 + \sin^2 \Delta \phi \right\},
\]
where \( \mathbf{v}_n = [e_n, e_{n+1}] \) is the vector product of \( e_n \) and \( e_{n+1} \) and \( h = \Delta z / R_0 \) is the dimensionless pitch of the helix. Below we will use the angle of rotation about the nth bond \( \delta_n = \pi - \eta_n \), where \( \eta_n \) is the nth dihedral angle. The equilibrium rotation angle is
\[
\delta_0 = \pi - \eta_0 = 16.32^\circ.
\]

Let \( x_n, y_n, z_n \) be the coordinates of the nth site in the helix chain. Passing from Cartesian to cylindrical coordinates, we obtain
\[
x_n = (R_0 + r_n) \cos(n \Delta \phi + \varphi_n)
\]
\[
y_n = (R_0 + r_n) \sin(n \Delta \phi + \varphi_n)
\]
\[
z_n = n \Delta z + h_n,
\]
where \( r_n, \varphi_n, \) and \( h_n \) are the radial, angular, and longitudinal displacements of the nth site from its equilibrium position, respectively. The Hamiltonian of the chain is
\[
H = \sum_n \left\{ \frac{1}{2} M \left[ \dot{r}_n^2 + \dot{\varphi}_n^2 (R_0 + r_n)^2 + \dot{h}_n^2 \right] + V(\rho_n) + U(\theta_n) + W(\delta_n) + S(r_n, u_n, v_n) \right\},
\]
where the dot denotes a derivative with respect to time \( t \), \( \rho_n \) is the length of the nth valence bond, \( \theta_n \) is the nth bond angle, and \( \delta_n \) is the nth rotation angle.

The potential of the nth valence bond is
\[
V(\rho_n) = D_0 \left[ 1 - \exp\left\{ -\alpha (\rho_n - \rho_0) \right\} \right]^2,
\]
where the length of the nth bond is
\[
\rho_n = [a_{n,1} + b_{n}^2]^{1/2}.
\]

Here,
\[
a_{n,1} = d_{n}^2 + d_{n+1}^2 - 2d_n d_{n+1} c_{n,1},
b_n = \Delta z + h_{n+1} - h_n,
d_n = R_0 + r_n,
c_{n,1} = \cos(\Delta \phi + \varphi_{n+1} - \varphi_n).
\]

According to [19], the valence bond energy is \( D = 334.72 \) kJ/mol and \( \alpha = 1.91 \) Å.

The deformation energy of the bond angle is
\[
U(\theta_n) = \frac{1}{2} K_0 \left[ \cos(\theta_n) - \cos(\theta_0) \right]^2,
\]
where the nth bond angle is
\[
\theta_n = \arccos\left\{ -(a_{n,2} + b_{n-1} b_n) / \rho_{n-1} \rho_n \right\}.
\]

Here,
\[
a_{n,2} = d_{n-1} d_n c_{n-1,1} + d_n d_{n+1} c_{n,1} + d_n^2 - d_{n-1} d_{n+1} c_{n,2} + c_{n,2} = \cos(2 \Delta \phi + \varphi_{n+1} - \varphi_{n-1})
\]

According to [20], we have \( K_0 = 529 \) kJ/mol.

The potential of internal rotation \( W(\delta_n) \) describes retardation of the chain units rotating about the nth valence bond. The nth rotation angle is
\[
\delta_n = \arccos\left\{ -(b_n b_{n+1} a_{n,2} + b_{n-1} b_n a_{n,1} + b_{n+1} a_{n,3} + b_{n-1} a_{n,3}) / \sqrt{\beta_n \beta_{n+1}} \right\},
\]
where
\[
a_{n,3} = d_n d_{n+2} s_{n-1,1} + d_n d_{n+1} s_{n,1} + d_n d_{n+1} s_{n,2} + d_n d_{n+2} s_{n,2} - d_n d_{n+1} c_{n,1},
\]
\[
a_{n,4} = d_n d_{n+2} c_{n-1,2} + d_n d_{n+1} c_{n,1} + d_n d_{n+2} c_{n,3} + d_n d_{n+1} c_{n,2} - d_n d_{n+1} c_{n,1},
\]
\[
s_{n,1} = \sin(\Delta \phi + \varphi_{n+1} - \varphi_n),
\]
\[
s_{n,2} = \sin(2 \Delta \phi + \varphi_{n+1} - \varphi_{n-1}),
\]
\[
s_{n,3} = \sin(3 \Delta \phi + \varphi_{n+2} - \varphi_{n-1})
\]
\[
\beta_n = a_{n-1,1} b_n^2 + a_{n,1} b_{n-1}^2 + b_{n-1} a_{n,2} + a_{n,2}.
\]

Figure 2 presents the form of the rotation potential for a PTFE macromolecule. A PTFE macromolecule has four rotation isomers per each C–C bond. Two of them \([\text{trans}(+)\) and \(\text{trans}(-)\)] have equal minimum energies \([\delta_l = \delta_t = 2 \pi - \delta_t, W(\delta_l) = W(\delta_t) = 0], \) and the
other two \(\text{[gauche}(+)\) and \(\text{gauche}(-)\)] have a higher energy \([\delta_3 = 2\pi/3, \delta_4 = 4\pi/3, W(\delta_3) = W(\delta_4) > 0]\).

The rotation potential is characterized by four parameters: the heights of the potential barriers between \(\text{trans}\)-conformations \(\epsilon_0 = W(0)\) and between \(\text{trans}\) and \(\text{gauche}\)-conformations \(\epsilon_1 = W(\pi/3)\), the energy of the \(\text{gauche}\)-conformation \(\epsilon_2 = W(2\pi/3)\), and the height of the potential barrier between \(\text{gauche}\)-conformations \(\epsilon_3 = W(\pi)\). According to [17], we have \(\epsilon_0 = 1.674\ \text{kJ/mol}, \epsilon_1 = 18.42\ \text{kJ/mol}, \epsilon_2 = 4.186\ \text{kJ/mol},\) and \(\epsilon_3 = 23.02\ \text{kJ/mol}\).

For the numerical modeling of the chain dynamics, it is convenient to define the rotation potential as

\[
W(\delta) = [C_1 Z_\alpha(\delta) + C_2 Z_\beta(\delta) - C_3]^2, \tag{4}
\]

where

\[
Z_\alpha(\delta) = \frac{(1 + \alpha)\sin^2(\delta/2)}{1 + \alpha\sin^2(\delta/2)}
\]

and

\[
Z_\beta(\delta) = \left[\frac{(1 + \beta)\sin(3\delta/2)}{1 - \beta\sin(3\delta/2)}\right]^2
\]

are the one-parameter functions.

The values of the parameters \(C_1 = 3.411\ \text{(kJ/mol)}^{1/2}, C_2 = 2.681\ \text{(kJ/mol)}^{1/2}, C_3 = 1.294\ \text{(kJ/mol)}^{1/2}, \alpha = 14.6125,\) and \(\beta = 4.0028 \times 10^{-3}\) are unambiguously determined from the system of equations

\[
W(0) = C_3^2 = \epsilon_0
\]

\[
W(\delta_0) = [C_1 Z_\alpha(\delta_0) + C_2 Z_\beta(\delta_0) - C_3]^2 = 0
\]

\[
W(\pi/3) = \left[C_1 \frac{1 + \alpha}{4 + \alpha} + C_2 \left(\frac{1 + \beta}{1 - \beta}\right)^2 - C_3\right]^2 = \epsilon_1
\]

\[
W(2\pi/3) = \left[3C_1 \frac{1 + \alpha}{4 + 3\alpha} - C_3\right]^2 = \epsilon_2
\]

\[
W(\pi) = (C_1 + C_2 - C_3)^2 = \epsilon_3.
\]

Figure 2 depicts the form of the potential given by Eq. (4) at the indicated values of the parameters. The potential has an absolute minimum at \(\delta = \delta_0\) and \(2\pi - \delta_0\).

The potential \(S(r_n, u_n, v_n)\) describes the interaction of the molecular chain with the substrate formed by the six neighbor chains. Its numerical value can be found by calculating the energy of interaction with the six immobile neighbor chains as a function of displacement of the chain. To do this, it is necessary to calculate the sum of the energies of nonvalence (van der Waals and Coulomb) interactions of all atoms and to divide it by the number of chain units.

Figure 2. The form of the rotation potential \(W(\delta)\) for a PTFE macromolecule.

Figure 3. Construction of dimensionless local coordinates \(u\) and \(v\) for a discrete helix. The solid lines correspond to units, and the circles indicate sites of a left-handed helix.

Let us introduce new local dimensionless coordinates

\[
u_n = (\varphi_n - h_n \Delta \phi/\Delta z)/2\pi \tag{5}
\]

\[
\varphi_n = u_n + h_n/\Delta z. \tag{6}
\]

The substrate potential is a two-dimensional periodic function of these variables: \(S(r, u \pm 1, v \pm 1) \equiv S(r, u, v)\). The region \(0 \leq u \leq 1, 0 \leq v \leq 1\) is a unit cell of the discrete helix (Fig. 3). Really, each \(n\)th helix unit occupies the site of the \((n - 1)\)th unit at \(u_n \equiv 1\) or the \((n + 1)\)th unit at \(v_n \equiv 1\). In both cases, the position of the infinite helix does not change. Therefore, it is sufficient to find the substrate potential only for the unit cell.
The substrate potential can be described analytically with a high accuracy by the double Fourier series

\[ S(r, u, v) = \frac{1}{2}K_{r}r^2 + b_{22}\cos[2\pi(u - v)] + \sum_{i=1}^{6} \sum_{j=1}^{6} a_{ij}\cos \{2\pi[(i - 1)(u - 1/2) + (j - 1)(v - 1/2)] \}, \]

where \( K_{r} \) is the transverse rigidity equal to 17.1 N/m, \( b_{22} = -0.075878 \text{ kJ/mol} \), and the values of other Fourier coefficients are as given in the table.

Figure 4 presents the two-dimensional plot of the substrate potential \( E = S(0, u, v) \). The bold line shows the most energetically preferred trajectory of the particle motion in the unit cell of the helix.

The Fourier coefficients for the analytical representation of the substrate potential (Eq. (7)) are as follows:

<table>
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<th>i</th>
<th>j</th>
<th>Value of ( a_{ij} ) (kJ/mol) at j</th>
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The small-amplitude vibrations of an isolated PTFE chain were analyzed in [16]. Two sonic velocities were revealed: \( v_l = 6978.6 \text{ m/s} \) is the velocity of long-wave longitudinal phonons and \( v_t = 5585.3 \text{ m/s} \) is the velocity of long-wave torsional phonons. The ratio of these velocities is \( s = v_t/v_l = 0.80035 \).

To find the stationary state of a topological defect (soliton) \( \{r_n, \varphi_n, h_n\}_{n=1}^{N} \) in a helical PTFE macromolecule, it is necessary to numerically solve the problem of the constrained minimum

\[ P = \sum_{n=1}^{N} \left\{ V(\rho_n) + U(\theta_n) + W(\delta_n) + S(r_m, u_m, v_m) \right\} \rightarrow \min \quad r_1 = 0, \quad \varphi_1 = \varphi_{\omega}, \quad h_1 = h_{\omega}, \quad \ldots, \quad r_N = 0, \quad \varphi_N = \varphi_{\omega}, \quad h_N = h_{\omega}. \]
and (10) in the dimensionless helical coordinates defined by Eqs. (5) and (6):

\[ r_1 = 0, \quad u_1 = 0, \quad 1, \quad v_1 = 0, \quad 1 \quad (11) \]

\[ r_N = 0, \quad u_N = 0, \quad 1, \quad v_N = 0, \quad 1. \quad (12) \]

Each of the boundary conditions (11) and (12) corresponds to a certain ground state of the chain. Therefore, the solution of the constrained-minimum problem (8) with (11), (12) corresponds to a certain ground state of the chain. Therefore, we are to numerically integrate the system of the equations of motion

\[ M\ddot{r}_n = M(R_0 + r_n)\phi_n^2 - \frac{\partial}{\partial r_n}P \]

\[ M(R_0 + r_n)^2\phi_n = -2M(R_0 + r_n)\phi_n\ddot{r}_n - \frac{\partial}{\partial \phi_n}P \quad (13) \]

\[ M\ddot{h}_n = -\frac{\partial}{\partial h_n}P \]

\[ n = 1, 2, \ldots, N \]

with the initial condition corresponding to a soliton with a charge of \( q_s = (-1, 1) \) and a velocity of \( v = 0.1v_t \), and to a stationary topological defect with other topological charge \( q_d \).

At \( q_s = (1, 0) \), collision of the soliton and the defect leads to a partial recombination resulting in that a stationary defect with the charge \( q = (0, 1) \) is left in the chain. The collision is accompanied by intense radiation of phonons. At \( q_s = (-1, 0) \), elastic reflection of the soliton from the defect occurs. The defect itself remains immobile. Elastic reflection also occurs at \( q_d = (0, 1) \) or \((-1, 1)\). In these cases, the defect also remains immobile. At \( q_d = (0, 1) \), a stationary defect with \( q = (-1, 0) \) is left in the chain as a result of partial relaxation. Partial recombination occurs also at \( q_d = (1, 1) \). In this case, a stationary defect with a double topological charge \( q = (0, 2) \) is left in the chain (Fig. 6). This means that stationary defects with multiple topological charges can exist in the chain.

A collision of two topological solitons of like charges always results in their elastic reflection, and a collision of two solitons of unlike charges leads to their complete recombination.

Numerical simulation of the dynamics of topological defects in a thermalized chain shows that, at \( T = 100 \) K, all the defects are stable to thermal vibrations of the chain. For defects with topological charge of \( q \neq \pm(1, 1) \), this stability is topological in origin: destruction of these defects requires removing half of the chain along the \( z \)-axis. The defect with a charge of \( q = \pm(1, 1) \) formed by local rotations of the helix units can be unstable towards thermal vibrations. At \( T = 100 \) K, this defect remained stable over the whole integration period \( t = 100 \) ps. Under the action of thermal vibra-
Fig. 5. The distribution of (a) radial $r_n$, (b) angular $\phi_n$, and (c) longitudinal $h_n$ displacements of the helix units and (d) the deformation energy of the chain $e_n$ ($n$ is the number of the chain unit) in the region of localization of a defect with a topological charge $q$ of (A) $(1, 0)$, (B) $(0, 1)$, (C) $(1, 1)$, and (D) $(-1, 1)$. The energy of the defect $E$ is (A) 52.4, (B) 33.6, (C) 28.9, and (D) 119.4 kJ/mol.
tions, the topological soliton (the defect with the charge $q = \pm (1, 1)$) moves like a free Brownian particle. Pinning of other topological defects is observed, so that their motion is reduced to rare thermally activated hops to neighbor units.

CONCLUSIONS

The present study of topological defects (solitons) in a PTFE crystal by numerical methods showed that, in a macromolecule taking the conformation of a three-dimensional helix, defects of the four types can exist. All the defects are stable to thermal vibrations of the chain. Each defect can be characterized by a two-dimensional topological charge. Defects of one type exhibit the soliton dynamics. They can move along the chain as a solitary wave. The velocity spectrum of these solitons falls in the subsonic range. Pinning of other defects is observed, and their motion has a character of thermally activated random hopping.

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