Original paper

Creation of mesoscale models of aged polymer nanoparticles using the Rosenbluth algorithm

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DOI: 10.26456/pcascnn/2026.18.428

Abstract: This paper presents a three-stage approach to constructing mesoscale models of aged polymer nanoparticles. The initial nanoparticle configuration is constructed using the lattice Rosenbluth algorithm, which has been adapted to address the current issue. This algorithm creates dense globules composed of a specified number of polymer chains, which are constructed from coarse-grained particles (beads) of a single type. Increasing the size of the nanoparticles, as determined by the number of beads they contain, results in increased polydispersivity of the polymer chains. This also results in increased shape anisotropy. For nanoparticles containing more than 100 beads, this anisotropy is preserved even after long-term relaxation, which is the second stage in the construction process. The third step involves transforming some beads into different types using a specific ratio. The type of bead, its location in the polymer chain, and its ratio are determined from literature sources. Some intra-chain bonds are broken, and new inter-chain bonds are formed. These changes form the basis of the nanoparticle aging algorithm. Applying the aging algorithm has been found to lead to the formation of large numbers of low-molecular-weight fragments inside nanoparticles. These degraded products easily desorb from nanoparticle surfaces into the surrounding environment.

Keyword: Rosenbluth algorithm, coarse-grained modeling, polymers, degradation, nanoparticles.

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УДК 544.23.022 *Оригинальная статья*

Построение мезомасштабных моделей состаренных полимерных наночастиц с использованием алгоритма Розенблута

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DOI: 10.26456/pcascnn/2026.18.428

Аннотация: В работе обсуждается трехступенчатая схема построения мезомасштабных моделей состаренных полимерных наночастиц. Построение начальной конфигурации наночастиц базируется на использовании решеточного алгоритма Розенблута, адаптированного к решаемой задаче. С его помощью создаются плотные глобулы, состоящие из заданного числа полимерных цепей, построенных из крупнозернистых частиц (бусин) одного типа. Увеличение размера наночастиц, определяемого числом бусин в их составе, приводит к росту

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полидисперсности полимерных цепей. Также при этом возрастает анизотропия формы, которая в случае наночастиц с числом бусин больше 100 сохраняется даже при использовании длительной релаксации (второй этап построения). На третьем этапе производилось преобразование части бусин в другие типы с использованием заданного соотношения. Типы бусин, их локализация в полимерных цепях и их соотношение определялись литературными данными. Также производился разрыв части связей внутри цепей и формировались новые межцепные связи. Совокупность этих преобразований составляет суть алгоритма старения наночастиц. Было обнаружено, что в результате применения алгоритма старения в составе наночастиц образуется большое число низкомолекулярных фрагментов. Такие продукты деградации могут легко десорбироваться с поверхности наночастиц в окружающую среду.
Ключевые слова: алгоритма Розенблута, крупномасштабное моделирование, полимеры, деградация, наночастицы.

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Поступила в редакцию/received: 27.07.2026; после рецензирования/revised: 30.08.2026; принята/accepted: 02.09.2026.

1. Introduction

Currently, there is a lot of attention being paid to the problem of environmental pollution by microplastic particles. These particles are formed when polymer waste is degraded by ultraviolet radiation, oxygen, water, and elevated temperatures [1-3]. During the aging process, polymers undergo several chemical changes: a decrease in molecular weight due to bond scission between monomer units of polymer chains; cross-link formation between chains; and oxygen-containing group accumulation (e.g., carbonyl and hydroperoxide groups). These changes cause morphological alterations in polymer products at the micro- and nanoscale [4, 5]. These processes result in the degradation and disintegration of the polymer structure into fragments whose size gradually decreases. This results in the formation of macroscopic particles as well as smaller micron- and nanoscale particles. As the particles become smaller, they can migrate long distances in aquatic environments and are found in remote regions of the planet, including fresh and marine water, the atmosphere, soil, and food. Due to chemical changes, aged polymer particles interact differently with biological systems [1, 3]. Because of their small size, micro- and nanoparticles (NPs) of aged polymers can be consumed by living organisms at different trophic levels. This raises concerns about the toxicological risks to biota and potential impacts on human health [1, 3]. It is believed that when these particles accumulate in the body, they can cause inflammation, allergic reactions, and asthma. Therefore, studying the aggregation and sedimentation processes of aged polymer particles in aquatic systems is a pressing issue.

Conducting reliable studies on the negative impact of aging nanoparticles requires manipulating particles at different stages of the aging process. However, laboratory experiments can only observe microscopic particles [6]. In this case, computer modeling can provide information on the properties of aged nanoparticles by allowing the study of processes at the atomic-molecular level [7]. Such studies require the ability to construct models of aged nanoparticles with a given number of polymer chains, their length, and chemical composition. For computer models to be highly reliable, aged NPs must be constructed in accordance with available experimental data.

This article discusses a method for constructing mesoscale models of aged nanoparticles (ANPs), taking into account the aging mechanisms described in [8-12]. The chosen concept involves creating polymer chains as linear sequences of structureless, spherical particles (beads) with the same diameter, σ. The beads are assigned different types to account for the chemical structure. This simplified construction allows us to develop a general method for constructing nanoparticles. We can then transform the resulting mesoscale models into all-atom representations using the reverse mapping concept by replacing the beads of each type with their associated all-atom model [13].

2. Algorithm for constructing nanoparticles of aged polymers

As mentioned above, using a mesoscale representation enables us to develop a general concept for creating aged polymer nanoparticles that meet specific parameters. First, we will formulate the requirements for the aged polymer nanoparticle model. By an «aged» nanoparticle model, we mean a set of polymer chains that have undergone chemical changes due to interaction with the environment. We believe such particles form due to polymer degradation, primarily from the accumulation of polymer chain scission within the material. This leads to the gradual disintegration of the intact material into individual fragments. Since disintegration begins in the amorphous regions of the polymer structure, we consider aged nanoparticles to be amorphous structures consisting of intertwined polymer chains. Key parameters of ANP models include the nanoparticle's molecular weight M, the total number of chains n_{chains}, the degree of polymerization n_{pol}, and the degree of polymer aging. It should be noted that the literature does not clearly define the concept of polymer aging degree. Based on general facts about polymer degradation processes [8-12], we will understand the aging degree as the percentage of chemically altered monomer units out of the total number of them. This characteristic may also include the number of chains within the ANP formed by the cleavage or formation of bonds between monomer units [11-12].

To simplify the process of constructing amorphous ANPs, we divide it into three stages. In the first stage, we generate a model of an amorphous

nanoparticle with a given molecular weight M consisting of n_{chains} with a degree of polymerization n_{pol}. This model is considered an unaged nanoparticle. At this stage, all chains are identical. In the second stage, we relax the prepared NP configuration in the framework of the Langevin dynamics. In the third stage, we modify the model by assigning types to selected chains that correspond to chemically modified monomers. It is also possible at this stage to adjust the chain lengths within the model and introduce interchain cross-links.

The main difficulty in creating models of polymer particles as entangled chains is that the nanoparticle itself is a dense system. For this reason, we believe the Rosenbluth method [14-15] is the most suitable. This method was initially proposed for modeling self-avoiding walks on regular lattices (e.g., square and simple cubic) to understand how polymers behave in solution when self-intersection between their monomer units is prohibited. The lattice nodes serve as sites for monomers, and the bonds between them represent chemical bonds in the chain. The key advantages of lattice models are their simplicity and computational efficiency. The original algorithm involves constructing a polymer chain as a sequence of «reasonable» local random steps rather than generating the entire configuration randomly. For our use case, we modified it so that the choice of direction is determined primarily by the energy gain from adding a new monomer unit. In other words, the direction with the lowest potential energy compared to the other directions is chosen. If there are multiple energetically advantageous directions, one is chosen at random.

Now, let's describe the developed construction scheme. Nanoparticle models are constructed from n_{chains} of linear polymers with a maximum degree of polymerization equal to n_{pol}. Thus, the total molecular mass M of the nanoparticle is n_{chains}, n_{pol}, i.e. $M = n_{chains} \cdot n_{pol}$. At the beginning of the creation process, a set of single beads equal to n_{chains}, which define the beginning of each chain, is randomly placed within a sphere with a radius of $(3M/4\pi)^{1/3}$. During construction, polymer chains are «grown» sequentially on a cubic lattice with a step of σ consisting of N^3 nodes. Each unsuccessful attempt n_{try} to add a new monomer unit to the selected chain is compared with the maximum number of attempts n_{trymax}. If $n_{try} > n_{trymax}$, the given chain is considered complete. This restriction is introduced to prevent the construction process from becoming looped. We also use a parameter, r_{max}, which is the maximum distance between chains that is taken into account when calculating the potential energy of the chain.

The following is a list of the steps for constructing a low-frequency model:

1. A chain is selected by generating a random number p from 1 to n_{chains}.

The termination of the algorithm is determined by the marking of all chains as complete (as indicated by chain flag FlagC).

2. The state of the construction completion flag FlagC is checked. If the chain is marked as complete, the algorithm proceeds to Step 1.

3. The number of false calls to this chain, n_{try}, is checked. If $n_{try} > n_{trymax}$, the chain is marked as complete and the algorithm proceeds to step 1.

4. The variable n_{try} is incremented by 1.

5. The energy $E(p)$ of the chain p is calculated:

$$E(p) = \sum_{p} \varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right], \; r_{ij} < r_{max}, \tag{1}$$

6. The summation is performed over all beads «i» belonging to the chain p, with all beads «j» inside the sphere $r_{ij} < r_{max}$.

7. One end of the chain is randomly selected and all adjacent, unoccupied nodes on the lattice are identified. If none are found, the other end of the chain is selected. If this end also has no adjacent unoccupied nodes, the chain is marked as «built» (FlagC = true) and is not considered further.

8. The chain energy, $E(p+k)$, is calculated by taking into account the addition of a new link at position k.

9. The difference $\Delta k = E(p+k) + E(p)$ is calculated.

10. Next, a following check is performed:

i) If there are several free nodes with $\Delta k < 0$ the position with the lowest Δk is selected.

ii) If there are several nodes with the same $\Delta k < 0$, the number of free nodes is selected randomly.

iii) If $\Delta k > 0$, a real number $Z \in [0,1)$ is generated, and if $\exp(-\Delta(k)) < threshold$, then k is accepted; otherwise, the transition to step 1 is performed. If there are several such positions, an attempt to place new bead is made for each of them.

11. A new monomer unit is placed in the selected position and a new bond is formed between it and the existing end unit. Then, the n_{try} variable is reset to zero.

12. If the length of the chain p is equal to n_{pol}, then the chain p is marked as «constructed» and not considered further.

13. The transition to step 1 is performed.

This algorithm is effective in terms of resource savings because it sharply reduces the number of unsuccessful attempts when modeling dense systems. Thus, by selecting the smallest contribution at each step, we obtain the most energetically favorable chain conformation.

Now, let us describe the algorithm for converting a constructed nanoparticle into an aged one, or the «aging» algorithm. When formulating the algorithm, we considered the following facts about the aging process of nanoparticles. According to modern concepts, changes in the structure of polymer chains and their chemical composition occur simultaneously during the aging process in polymeric materials [8-12]. The number and position of chemically modified groups depend on the degree of aging, which is determined by time, and on the type of polymer. The current implementation of the «aging» algorithm was performed for polyethylene (PE). We selected monomer units containing vinyl, acid, ketone, aldehyde, γ-lactone, and ester groups as possible chemically modified monomer units of the aged PE chain. These monomer units were assigned their own beads in the aged chain model. Due to the peculiarities of the PE chain degradation process, monomer units containing vinyl, aldehyde, and acid groups can only be located at the ends of polymer chains. In this case, the number of vinyl and acid groups is assumed to be equal. Monomer units with ketone, ester, and γ-lactone groups can only be found within the polymer chain.

We introduce the number of cross-links n_{clinks} as an additional parameter in the transformation of the prepared polymer nanoparticle. These cross-links are formed between monomer units with unsaturated bonds as result of splitting off hydrogen atom, which occurs either by absorbing a light quantum or due to capturing by the peroxide group of an adjacent chain. The number of radicals formed depends on the UV exposure time and the oxygen concentration in the material. Thus, in our model n_{clinks} is an open parameter and we only consider the formation of cross-links between the original PE monomer units.

Based on these considerations, we developed the following algorithm for transforming PE nanoparticles into aged ones:

1. The number of chemically modified monomer units containing each type of functional group (i.e., vinyl, acid, ketone, aldehyde, γ-lactone, and ester, for a total of N_a) is specified, as well as the number of cross-links n_{clinks}.

2. The chain that contains acid, aldehyde, or vinyl groups at it terminal monomer units is randomly selected.

3. If there are insufficient terminal units, randomly selected bonds in randomly selected chains are broken, and the acid, aldehyde, and vinyl groups are distributed among the resulting terminal monomers. This step is repeated until the specified number of monomer units with these groups is reached. If the specified value is not reached within 10^3 steps, an error message is generated.

4. The remaining starting monomers are randomly selected to distribute the remaining types of chemical groups. If the specified value is not reached within 10^3 steps, an error message is generated.

5. By randomly selecting pairs of initial monomers located on adjacent nodes, we form cross-links until the specified number of n_{clinks} is reached. If the specified value is not reached within 10^3 steps, an error message is generated.

As an additional step in constructing the NPs, we employed a relaxation procedure within the Langevin dynamics method [16, 17]. The relaxation protocol was taken from [18]. It included the following steps:

1. The prepared model is placed in a cubic simulation cell with periodic boundary conditions enabled and an edge length of $L \approx 2M\sigma$.

2. The NPs are relaxed. The interaction potential multiplier (1) for monomer units corresponding to unchanged monomer units, as well as for vinyl and crosslinked units, was increased from $\varepsilon_{AA} = 0{,}1\,k_BT$ to $\varepsilon_{AA} = 1{,}31\,k_BT$ in increments of 0,01 over $2 \cdot 10^6$ Langevin dynamics (LD) integration steps.

Below there are specific examples of using our NP construction scheme.

3. Results

The developed algorithms were used to create coarse-grained models of aged polymer nanoparticles. Fig. 1 a, 1 b, and 1 c (first column) show examples of polymer nanoparticles with a total number of beads of M = 600 (five chains), 20 584 (five chains), and 55 809 (ten chains), respectively. Fig. 1 (column 1) shows the general appearance of the constructed nanoparticles. As can be seen, the irregular shape of the nanoparticles is due to the restrictions, imposed by the cubic lattice on which the nanoparticles are constructed, on the choice of possible coordinates of new beads when they are added to a chain.

Fig. 2 shows the chain length distributions within the nanoparticles by green bars. As the nanoparticle size increases, the polydispersity of the chains within them also increases. For the smallest nanoparticle, all chains are the same length. For the second nanoparticle, only three chains have the same length. For the largest nanoparticle, all chains have distinct lengths. Thus, the parameter n, which sets the chain size limit, is not reached as the nanoparticle size increases. This occurs when all lattice sites near the growing end of a chain are occupied. Therefore, it is impossible to construct large nanoparticles based on long, identical chains.

The obtained initial NP configurations were relaxed over $2 \cdot 10^6$ LD steps. During this process, the shape of the NPs gradually smoothed out. In all cases, we did not observe the NPs transitioning to a spherically symmetric morphology. This transition is hindered by the entanglement of polymer chains. Next, the constructed NPs were aged. The degree of aging was set equal to 25% based on the number of chemically modified groups.

As Fig. 3 shows, the relative number of chemically modified groups remains stable for NPs of the considered sizes. At the same time, the fraction of low-molecular fragments (oligomeric chains shorter than 20 monomer units) in

the NP composition increased dramatically (see Fig. 2).

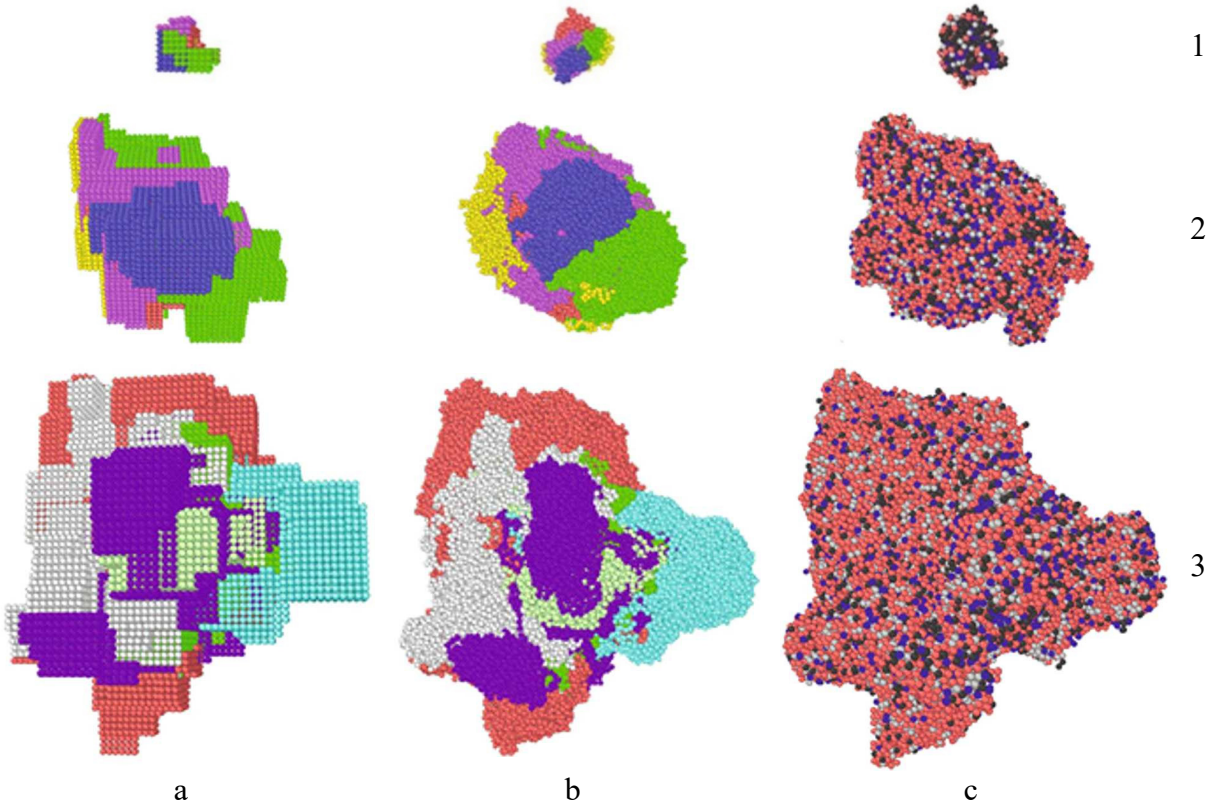

Fig. 1. Examples of the results of constructing coarse-grained models of nanoparticles with: (a) M = 600, (b) 20 584 and (c) 55 809. The column numbers correspond to the following stages of construction: (1) the type of NP after the completion of the algorithm (all beads are ordered on a cubic lattice), (2) the type of NP after the completion of the equilibration procedure using the LD method, (3) the type of NP after the completion of the aging procedure (25% of chemically modified monomer units). The coloring of the beads in columns (1) and (2) shows their belonging to different chains. In column (3), the coloring of the beads determines: red - the original monomer units, black - units containing vinyl groups, blue - containing oxygen-containing groups and gray - beads between which cross-links are introduced.

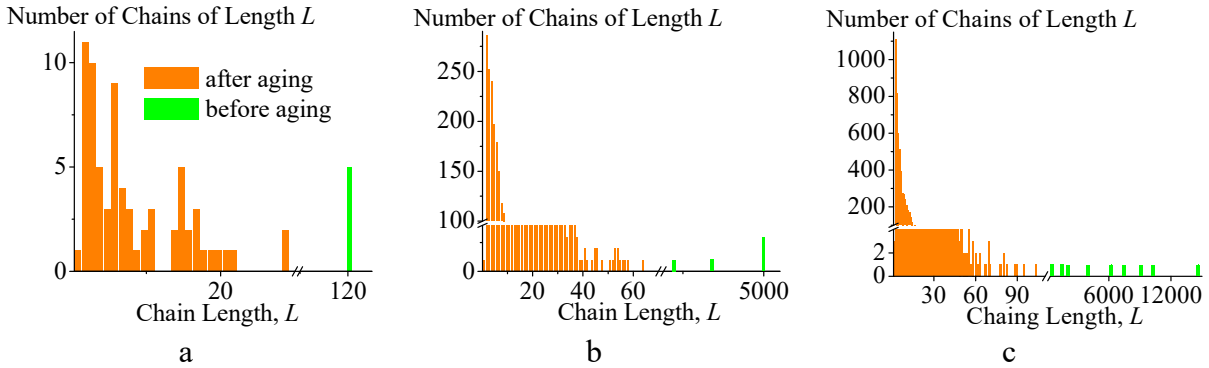

Fig. 2: Chain length distribution of nanoparticles consisting of 600 beads (a), 20 584 beads (b), and 55 809 beads (c). Green indicates the original (unaged) nanoparticles, while red shows the length distribution after applying the aging algorithm.

Note that the formation of these fragments is due to the random nature of

polymer chain rupture in the NP aging model. According to Fig. 2, as M increases, the chain length distribution tends to normalize. If the presence of low-molecular fragments is undesirable in a computer experiment based on the conditions of the problem being solved, they can be removed from the model by introducing additional steps into the calculation scheme.

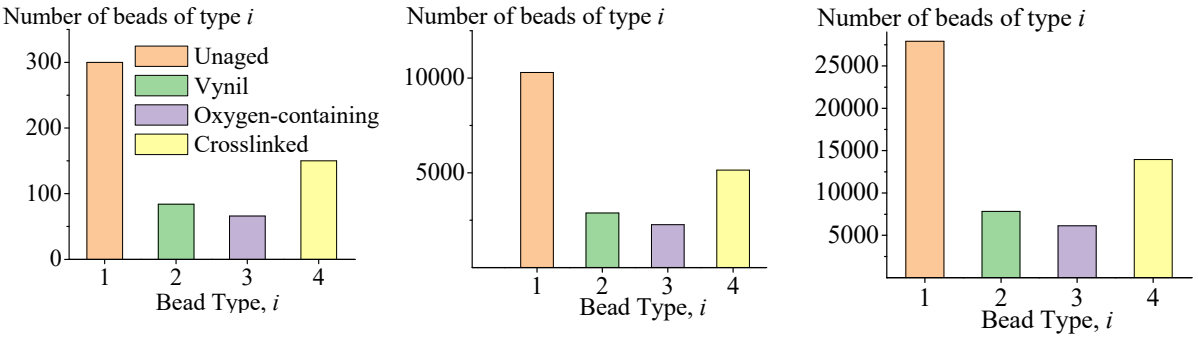

Fig. 3. The number of chemically modified beads in aged NPs with 600 beads (a), 20 584 beads (b), and 55 809 beads (c) after completing the aging procedure.

4. Conclusion

We developed a three-stage scheme for constructing aged polymer nanoparticles based on an adapted lattice algorithm for polymer chain construction and on the existing literature on polymer chemical transformations resulting from exposure to ultraviolet radiation, oxygen, water, and temperature. Using this computational scheme, we constructed a series of NP models. We found that, when using parameter values $n_{pol} > 100$, the degree of polydispersity of the polymer chains increases with an increase in the total number of beads in the NPs. Also, in this case the anisotropy of the NP shape increases and is preserved even with prolonged NP relaxation. Furthermore, the aging procedure allows the creation of NPs with a well-maintained relative content of chemically modified groups. The resulting chain length distributions of the NPs produced by the aging procedure result in a significant proportion of low-molecular-weight fragments. According to [18], such oxygen-containing monomer unit degradation products can easily desorb from the surface of nanoparticles and pass into the aqueous medium. This process can contribute to a further reduction in the molecular weight of the NPs during aging.

A test calculations were carried out using equipment from the National Research Center «Kurchatov Institute» (http://ckp.nrcki.ru/), the main calculations were carried out using equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University [19].

This research was funded by the Ministry of Science and Higher Education of the Russian Federation (state contract no. 075-15-2025-016, MegaGrant).

References:

1. Kim M.-S. Modeling study on fate of micro/nano-plastics in micro/nano-hydrodynamic flow of freshwater, *Journal of Hazardous Materials,* 2021, vol. 419, art. no. 126397, 14 p. DOI: 10.1016/j.jhazmat.2021.126397.
2. Martín J., Santos J.L., Aparicio I., Alonso E. Microplastics and associated emerging contaminants in the environment: Analysis, sorption mechanisms and effects of co-exposure, *Trends in Environmental Analytical Chemistry*, 2022, vol. 35, art. no. e00170, 15 p. DOI: 10.1016/j.teac.2022.e00170.
3. Hoseini M., Stead J., Bond T. Ranking the accelerated weathering of plastic polymers, *Environmental Sciences: Processes and Impacts*, 2023, vol. 25, issue 12, pp. 2081-2091, DOI: 10.1039/d3em00295k.
4. Shyichuk A.V., White J.R., Craig I.H., Syrotynska I.D. Comparison of UV-degradation depth-profiles in polyethylene, polypropylene and an ethylene–propylene copolymer, *Polymer Degradation and Stability*, 2005, vol. 88, pp. 415-419, DOI: 10.1016/j.polymdegradstab.2004.12.006.
5. White J.R., Shyichuk A.V. Macromolecular scission and crosslinking rate changes during polyolefin photo-oxidation, *Polymer Degradation and Stability*, 2007, vol. 92, issue 7, pp. 1161-1168, DOI: 10.1016/j.polymdegradstab.2007.04.011.
6. Ruan X., Xie L., Liu J. et al. Rapid detection of nanoplastics down to 20 nm in water by surface-enhanced Raman spectroscopy, *Journal of Hazardous Materials,* 2024, vol. 462, art. no. 132702, 10 p. DOI: 10.1016/j.jhazmat.2023.132702.
7. Roy S., Bhattacharjee J. Nano-scale computational modeling: challenges, limitations, and emerging trends, *Advanced Nanomaterials in Biomedical Implants: Processing, Structures, Properties and, Applications*. Amsterdam, Elsevier, 2025, pp. 471-494, DOI: 10.1016/B978-0-443-27378-0.00018-0.
8. Ranby B.G., Rabek J.F. *Photodegradation, photo-oxidation, and photostabilization of polymers: principles and applications*. London, John Wiley & Sons, 1975, 590 p.
9. Adams J.H. Analysis of nonvolatile oxidation products of polypropylene. III. Photodegradation, *Journal of Polymer Science. Part A1,* 1970, vol. 8, issue 5, pp. 1279-1288, DOI: 10.1002/pol.1970.150080520.
10. Costa, L., Luda M.P., Trossarelli L. Ultra-high molecular weight polyethylene – II. Thermal- and photo-oxidation, *Polymer Degradation and Stability*, 1997, vol. 58, issue 1-2, pp. 41-54, DOI: 10.1016/s0141-3910(97)00010-4.
11. Wu Q., Qu B., Xu Y., Wu Q. Surface photo-oxidation and photostabilization of photocross-linked polyethylene, *Polymer Degradation and Stability*, 2000, vol. 68, issue 1, pp. 97-102, DOI: 10.1016/s0141-3910(99)00171-8.
12. Gardette M., Perthue A., Gardette J.-L. et al. Photo- and thermal-oxidation of polyethylene: Comparison of mechanisms and influence of unsaturation content, *Polymer Degradation and Stability,* 2013, vol. 98, issue 11, pp. 2383-2390, DOI: 10.1016/j.polymdegradstab.2013.07.017.
13. Scacchi A., Vuorte M., Sammalkorpi M. Multiscale modelling of biopolymers, *Advances in Physics: X,* 2024, vol. 9, issue 1, art. no. 2358196, 55 p. DOI: 10.1080/23746149.2024.2358196.
14. Hsu H.-P., Grassberger P. A review of Monte Carlo simulations of polymers with PERM, *Journal of Statistical Physics*, 2011, vol. 144, pp. 597-637, DOI: 10.1007/s10955-011-0268-x.
15. Binder K., Paul W. Recent developments in Monte carlo simulations of lattice models for polymer systems, *Macromolecules*, 2008, vol. 41, issue 13, pp. 4537-4550, DOI: 10.1021/ma702843z.
16. Paquet E., Viktor H.L. Molecular dynamics, Monte Carlo simulations, and Langevin dynamics: A computational review, *Biomed Research International*, 2015, vol. 2015, art. no. 183918, 18 p. DOI: 10.1155/2015/183918.
17. Liwo A., Czaplewski C., Sieradzan A.K. et al. Theory and practice of coarse-grained molecular dynamics of biologically important systems, *Biomolecules*, 2021, vol. 11, art. no. 1347, 31 p. DOI: 10.3390/biom11091347.
18. Glagolev M., Volgin I., Malyshev M. et al. Probing the structural evolution and stability of aged polyethylene nanoparticles through coupled atomistic-mesoscale simulations, *Macromolecules*, 2026, vol. 59, issue 12, pp. 6629-6643, DOI: 10.1021/acs.macromol.6c00213.
19. Voevodin Vl., Antonov A., Nikitenko D. et. al. Supercomputer Lomonosov-2: large scale, deep monitoring and fine analytics for the user community, *Supercomputing Frontiers and Innovations*, 2019, vol. 6, issue 2, pp. 4-11. DOI: 10.14529/jsfi190201.

Библиографический список:

1. **Kim, M.-S.** Modeling study on fate of micro/nano-plastics in micro/nano-hydrodynamic flow of freshwater / M.-S. Kim // Journal of Hazardous Materials. – 2021. – V. 419. – Art. № 126397. – 14 p. DOI: 10.1016/j.jhazmat.2021.126397.
2. **Martín, J.** Microplastics and associated emerging contaminants in the environment: Analysis, sorption

mechanisms and effects of co-exposure / J. Martín, J.L. Santos, I. Aparicio, E. Alonso // Trends in Environmental Analytical Chemistry. – 2022. – V. 35. – Art. № e00170. – 15 p. DOI: 10.1016/j.teac.2022.e00170.
3. **Hoseini, M.** Ranking the accelerated weathering of plastic polymers / M. Hoseini, J. Stead, T. Bond // Environmental Science: Processes and Impacts. – 2023. – V. 25. – I. 12. – P. 2081-2091. DOI: 10.1039/d3em00295k.
4. **Shyichuk, A.V.** Comparison of UV-degradation depth-profiles in polyethylene, polypropylene and an ethylene–propylene copolymer / A.V. Shyichuk, J.R. White, I.H. Craig, I.D. Syrotynska // Polymer Degradation and Stability. – 2005. – V. 88. – P. 415-419. DOI: 10.1016/j.polymdegradstab.2004.12.006.
5. **White, J.R.** Macromolecular scission and crosslinking rate changes during polyolefin photo-oxidation / J.R. White, A.V. Shyichuk // Polymer Degradation and Stability. – 2007. – V. 92. – I. 7. – P. 1161-1168. DOI: 10.1016/j.polymdegradstab.2007.04.011.
6. **Ruan, X.** Rapid detection of nanoplastics down to 20 nm in water by surface-enhanced Raman spectroscopy / X. Ruan, L. Xie, J. Liu et al. // Journal of Hazardous Materials. – 2024. – V. 462. – Art. № 132702. – 10 p. DOI: 10.1016/j.jhazmat.2023.132702.
7. **Roy, S.** Nano-scale computational modeling: challenges, limitations, and emerging trends / S. Roy, J. Bhattacharjee // Advanced Nanomaterials in Biomedical Implants: Processing, Structures, Properties and, Applications. – Amsterdam: Elsevier, 2025. – P. 471-494. DOI: 10.1016/B978-0-443-27378-0.00018-0.
8. **Ranby, B.G.** Photodegradation, photo-oxidation, and photostabilization of polymers: principles and applications / B.G. Ranby, J.F. Rabek. – London: John Wiley & Sons, 1975. – 573 p.
9. **Adams, J.H.** Analysis of nonvolatile oxidation products of polypropylene. III. Photodegradation / J.H. Adams // Journal of Polymer Science Part A-1: Polymer Chemistry. – 1970. – V. 8. – I. 5. – P. 1279-1288. DOI: 10.1002/pol.1970.150080520.
10. **Costa, L.** Ultra-high molecular weight polyethylene – II. Thermal- and photo-oxidation / L. Costa, M.P. Luda, L. Trossarelli // Polymer Degradation and Stability. – 1997. – V. 58. – I. 1-2. – P. 41-54. DOI: 10.1016/s0141-3910(97)00010-4.
11. **Wu, Q.** Surface photo-oxidation and photostabilization of photocross-linked polyethylene / Q. Wu, B. Qu, Y. Xu, Q. Wu // Polymer Degradation and Stability. – 2000. – V. 68. – I. 1. – P. 97-102. DOI: 10.1016/s0141-3910(99)00171-8.
12. **Gardette, M.** Photo- and thermal-oxidation of polyethylene: Comparison of mechanisms and influence of unsaturation content / M. Gardette, A. Perthue, J.-L. Gardette et al. // Polymer Degradation and Stability. – 2013. – V. 98. – I. 11. – P. 2383-2390. DOI: 10.1016/j.polymdegradstab.2013.07.017.
13. **Scacchi, A.** Multiscale modelling of biopolymers / A. Scacchi, M. Vuorte, M. Sammalkorpi // Advanced Physics X. – 2024. – V. 9. – I. 1. – Art. № 2358196. – 55 p. DOI: 10.1080/23746149.2024.2358196.
14. **Hsu, H.-P.** A review of Monte Carlo simulations of polymers with PERM / H.-P. Hsu, P. Grassberger // Journal of Statistical Physics. – 2011. – V. 144. – P. 597-637. DOI: 10.1007/s10955-011-0268-x.
15. **Binder, K.** Recent developments in Monte Carlo simulations of lattice models for polymer systems / K. Binder, W. Paul // Macromolecules. – 2008. – V. 41. – I. 13. – P. 4537-4550. DOI: 10.1021/ma702843z.
16. **Paquet, E.** Molecular dynamics, Monte Carlo simulations, and Langevin dynamics: A computational review / E. Paquet, H.L. Viktor // Biomedical Research International. – 2015. – V. 2015. – Art. № 183918. – 18 p. DOI: 10.1155/2015/183918.
17. **Liwo, A.** Theory and practice of coarse-grained molecular dynamics of biologically important systems / A. Liwo, C. Czaplewski, A.K. Sieradzan et al. // Biomolecules. – 2021. – V. 11. – I. 9. – Art. № 1347. – 31 p. DOI: 10.3390/biom11091347.
18. **Glagolev, M.** Probing the structural evolution and stability of aged polyethylene nanoparticles through coupled atomistic-mesoscale simulations / M. Glagolev, I. Volgin, M. Malyshev et al. // Macromolecules. – 2026. – V. 59. – I. 12. – P. 6629-6643. DOI: 10.1021/acs.macromol.6c00213.
19. **Voevodin, Vl.** Supercomputer Lomonosov-2: large scale, deep monitoring and fine analytics for the user Community / Vl. Voevodin, A. Antonov, D. Nikitenko et. al. // Supercomputing Frontiers and Innovations. – 2019. – V. 6. – I. 2. – P. 4-11. DOI: 10.14529/jsfi190201.