Original paper

Development of a computational model for stability assessment of N-vinylcaprolactam – N-vinylimidazole copolymers in a selective solvent

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Abstract: Computer simulation of the behavior of thermosensitive copolymers of *N*-vinylcaprolactam and *N*-vinylimidazole in a water environment was performed using a pipeline of unidirectionally coupled simulation models, namely Dissipative Particle Dynamics, Langevin Dynamics, and All-atom Molecular Dynamics. The pipeline allows first to determine a possible sequence of monomer units in a model copolymer, then to determine the morphology of the globules formed in a selective solvent, and finally to assess the aggregation stability of the globules. It utilizes the fast relaxation dynamics in Dissipative Particle Dynamics Simulations, efficiency of implicit solvent consideration in Langevin dynamics, and experimentally verified atom interaction force-field in All-atom Molecular dynamics simulations. The approach exploits the strengths of each of the simulation methods, and the relevance of the simulation results is ensured by the ultimate transition to the all-atom detailed representation. Here we describe the models and the algorithms of transformation between the models, and present the data for their initial validation. The behavior of the studied models in an aqueous environment allows us to conclude that the constructed systems are structurally stable. The globules have a distinct core-shell structure, with *N*-vinylcaprolactam monomer units forming the core and *N*-vinylimidazole monomer units forming the outer shell. Water molecules penetrate the globule primarily through the shell, which is rich in *N*-vinylimidazole units.

Keywords: poly(N-vinylcaprolactam), poly(N-vinylimidazole), thermosensitive copolymers, computer simulation, thermally-switched catalysts.

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Разработка компьютерной модели для оценки стабильности сополимеров *N*-винилкапролактама – *N*-винилимидазола в селективном растворителе

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Аннотация: Изучение поведения термочувствительных сополимеров *N*-винилкапролактама и *N*-винилимидазола в водной среде было выполнено с использованием цепочки сопряженных компьютерных моделей на основе: метода диссипативной динамики частиц, Ланжевеновской динамики и полноатомной молекулярной динамики. Такой подход позволяет на первом этапе

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определить возможную последовательность мономерных звеньев в модельном сополимере, затем установить морфологию глобул, образующихся в селективном растворителе, и, на третьем этапе оценить структурную устойчивость данных глобул. Используются быстрая релаксация в методе диссипативной динамики частиц, эффективность неявного рассмотрения растворителя в методе Ланжевеновской динамики, и параметризованные по экспериментальным данным силовые поля в методе полноатомной молекулярной динамики. Таким образом, подход использует сильные стороны каждого из методов моделирования, а достоверность результатов обеспечивается за счет перехода на конечном этапе к детальному полноатомному описанию. В данной работе описаны используемые модели и алгоритмы преобразования моделей, и представлены данные их предварительной валидации. Поведение исследуемых моделей в водной среде позволяет сделать вывод о структурной стабильности построенных систем. Глобулы имеют ярко выраженную структуру типа «ядро-оболочка», где мономерные звенья *N*-винилкапролактама образуют ядро, а мономерные звенья *N*-винилимидазола — внешнюю оболочку. Проникновение молекул воды в глобулу происходит преимущественно через оболочку, богатую звеньями *N*-винилимидазола.
Ключевые слова: поли(N-винилкапролактам), поли(N-винилимидазол), термочувствительные сополимеры, компьютерное моделирование, термопереключаемые катализаторы

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1. Introduction

Stimuli-responsive polymers are a class of macromolecular systems that can undergo reversible transitions upon the change of external conditions, such as temperature, pH, salinity or radiation [1]. They can be used as a basis for sensors [2], tunable surfaces [3], and thermo-switchable catalysts. The latter can be based on thermosensitive polymers with lower critical solution temperature (LCST) [4-6], including copolymers of N-vinylcaprolactam (VCL) and N-vinylimidazole (VI).

The VCL-VI copolymers have been synthesized using the radical polymerization in solution [7-9] and in monomer feed [10-12]. Stimuli-responsive copolymers of N-vinylcaprolactam and N-vinylimidazole have been recently explored as a prospective basis for smart catalysis systems. An efficient way to synthesize them using the free-radical copolymerization in a monomer mixture was recently proposed by Barabanova and co-authors [10, 12]. It has been shown that at least at certain concentrations the copolymers, obtained from a monomer feed containing 85% VCL and 15% VI, can exhibit so-called protein-like (PL) behavior [12], i.e., upon heating the aqueous media, which renders it a poor solvent for the VCL monomer units of the copolymer, they undergo a conformational transition without precipitating from the solution. This

behavior is rather unexpected in polymers obtained using the one-pot synthesis.

To understand the emergence of PL behavior, one has to look into the supramolecular self-organization of the polymers. This can be achieved by computer simulation of a model copolymer in a selective solvent. Because experimental methods are unable to reliably determine the patterns of the monomer unit distribution along the polymer backbone, one can use a model of the copolymerization process, reproducing the synthesis conditions and the relevant factors, affecting the distribution. Taking into account large numbers of monomer units involved, the most suitable approach is the Dissipative Particle Dynamics (DPD) [13, 14]. It allows obtaining polymer chains with molecular masses similar to those observed in the experiment. On the other hand, Langevin dynamics (LD) [15, 16] allows simulating the evolution of the system without taking into account the solvent molecules, which greatly accelerates the computation. At the same time, the aggregational stability of the polymer systems can be reliably predicted only using All-Atom (AA) models [17, 18]. With the relaxation performed in the LD framework, the AA simulations can reach the equilibrium structure within achievable simulation times. The interaction potentials used in the AA models are parameterized and fine-tuned using large volumes of experimental data, enabling them to accurately reproduce the experimentally observed system behavior. The proposed chain of models thus utilizes the advantages of all of the methods: the explicit representation of all of the monomer units and fast relaxation dynamics of DPD, the efficiency of implicitly considering the solvent molecules in LD, and the accuracy of AA interaction force-field.

Here we report the development of such a model chain, and report the initial stability assessment of polymer globules, obtained from a simulated monomer mixture containing 85% of VCL and 15% of VI, which revealed protein-like behavior in the experimental study [12].

2. Models and simulation techniques

The preparation of the model systems and the simulations were conducted in 4 consecutive stages. At the first stage, the simulation of the reaction of radical copolymerization in the monomer feed was simulated using the DPD approach [14]. At the second stage, the obtained model copolymer chains were simulated in the selective solvent using the LD approach [16]. At the third stage, the globular structures obtained in LD were converted from mesoscale to all-atom representation and placed into an aqueous environment. At the final stage, the constructed system was subjected to a prolonged relaxation using all-atom molecular dynamics and a Class II PCFF force-field [19]. After the relaxation, the properties of the systems were calculated during production runs. The DPD, LD and AA simulations were performed using LAMMPS [20]. Below we

outline the details of each stage.

The simulation of the synthesis of VCL-VI copolymers in the monomer feed was performed using reaction DPD [21]. Unlike the earlier model [22], where the synthesis of the VCL-VI copolymers was performed in a solution, we used 3 types of particles, corresponding to the VCL and VI monomers, and the AIBN reaction initiator.

During the DPD simulations, the chemical bonds between the monomer units were formed every $n = 100$ equations of motion integration steps, which was sufficient for the polymer chain relaxation. The «bond/react» fix [23, 24] supplied with LAMMPS was employed. The probabilities of the covalent bond formation were chosen based on the experimentally determined copolymerization constants of VCL and VI [10]. The probabilities were derived from the following relationships: $r_{VCL} = w_{VCL,VCL} / w_{VCL,VI}$, $r_{VI} = w_{VI,VI} / w_{VI,VCL}$, and $w_{VCL,VI} = w_{VI,VCL}$. The pairwise interactions of the monomers were parameterized based on Groot-Warren parameterization of DPD interactions [14], and the value of the interaction potential factor $a_{VCL,VI}$ between VCL and VI was taken from our previous study [22].

The initial configurations were generated by randomly placing 4 AIBN initiator molecules and 46871 monomer molecules in a simulation cell with an edge size of 25σ. The σ is the DPD length unit corresponding to an average comonomer size of 4,5Å. The fraction of VCL monomer units was 85%. The copolymerization process was started after a relaxation run of 1000000 DPD simulation steps.

After reaching the target monomer conversion (q), the monomer unit sequences of the generated chains were determined, and the chains were recreated for LD simulations as random coils using MOUSE2 toolkit [25]. The generated chains were placed in simulation cells with an edge size from 1000σ to 4000σ, depending on the chain length, to simulate the structuring in a selective solvent. The LD simulation protocol was identical to that used in our previous study [10]. During the LD simulation stage, dense globules with a core-shell structure were obtained.

To switch to the all-atom representation, a reverse-mapping procedure developed by us was applied. The procedure involved scaling the model copolymer globules by a factor of $\sigma = 4{,}5$, replacing the coarse-grained structureless monomer units with all-atom models of the monomers (see Fig. 1), and determining the covalent bonds between the carbon atoms of the backbone. The open valences were filled by linking hydrogen atoms to the terminal units of each chain. The converted nanoparticles were placed in a spherical void inside a simulation cell with an edge length of 100 Å, filled with water molecules with a density of 1 g/cm^3, and the geometry of the system was optimized. As a result,

the all-atom polymer structures in an aqueous medium were obtained.

The MD simulations were performed in a NPT ensemble at $T = 323$ K, at which the water is a poor solvent for VCL, and a pressure of $P = 1$ bar, maintained by a Nose-Hoover thermostat/barostat, with a relaxation constants of 1 ps and 2 ps for the thermostat and barostat respectively. The integration step was 1 fs. Long-range Coulomb interactions were calculated using PPPM. The cutoff radius of the Van-der-Waals interactions was 18 Å. The relaxation of the AA models was performed for 10 ns. The consequent trajectory processing allowed obtaining data on density distributions for different types of atoms, numbers of hydrogen bonds between the globules and the water molecules, and the surface area of VCL units accessible to the solvent.

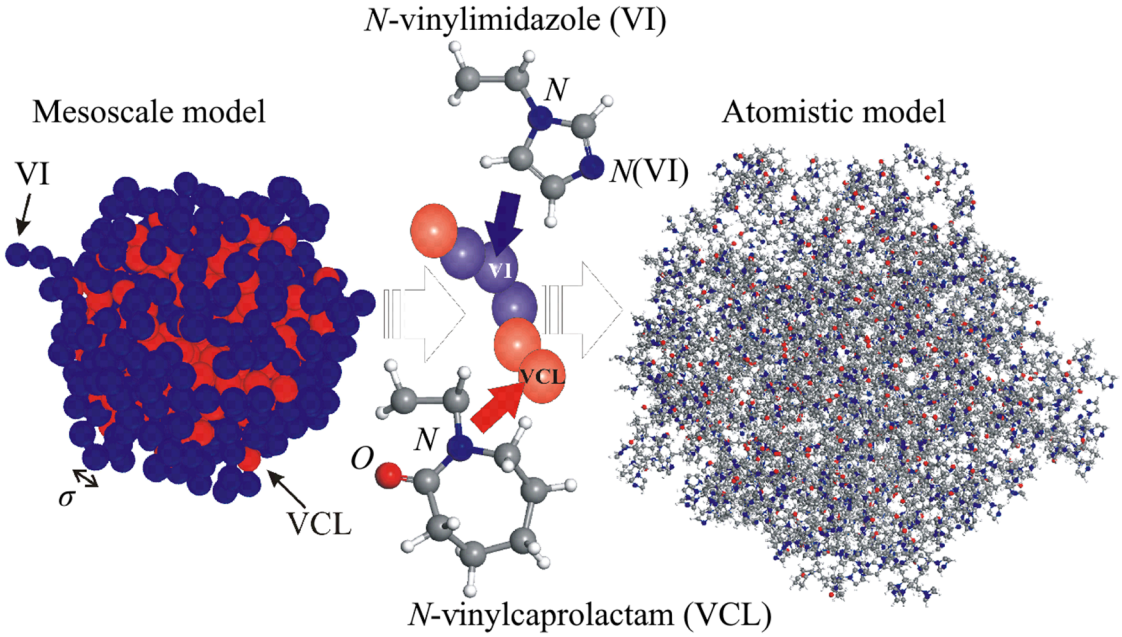

Fig. 1. Schematic representation of reverse-mapping of a collapsed VCL-VI copolymer chain (left) into all-atom representation (right) by replacing the mesoscopic beads with the corresponding all-atom monomer units of VCL and VI.

3. Results

The globules designated as «globule1» and «globule2» with the numbers of particles of 14709 and 13202, were constructed using the algorithm described above. Taking into account the water molecules, the total number of atoms in the systems was 112086 and 110816, correspondingly. The molecular mass and composition of the obtained copolymer chains corresponded to the samples studied in [12], which have demonstrated protein-like behavior at a concentration of 0,1 mg/mL.

The radius of gyration of the globules as a function of time is shown in Fig. 2. One can see that the structure is instantly stabilized, and after the initial swelling the gyration radii of the globules are constant. The obtained dependencies thus indicate the structural stability of the all-atom models of the globular aggregates constructed by transforming the coarse-grained models.

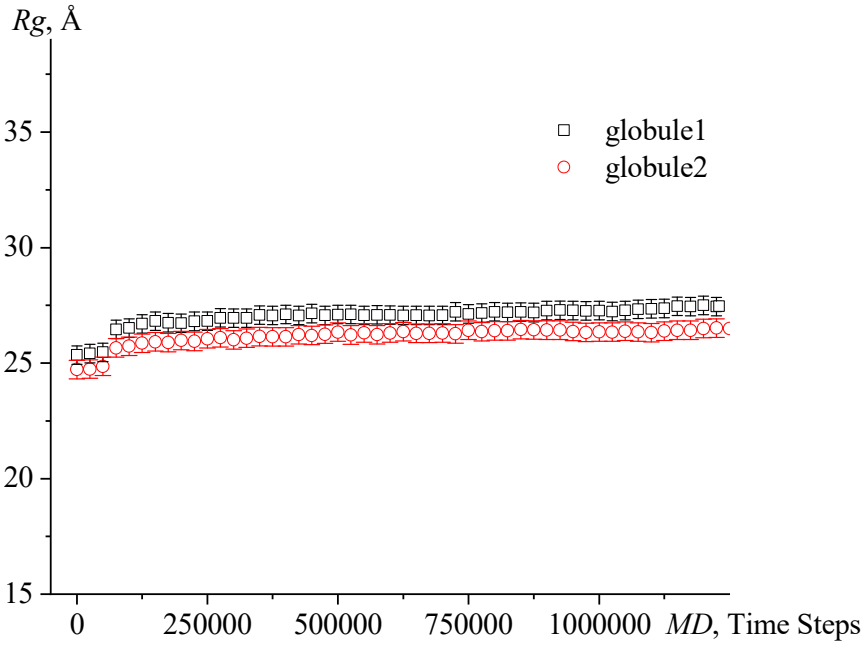

Fig. 2. Radius of gyration of the constructed globules as a function of time.

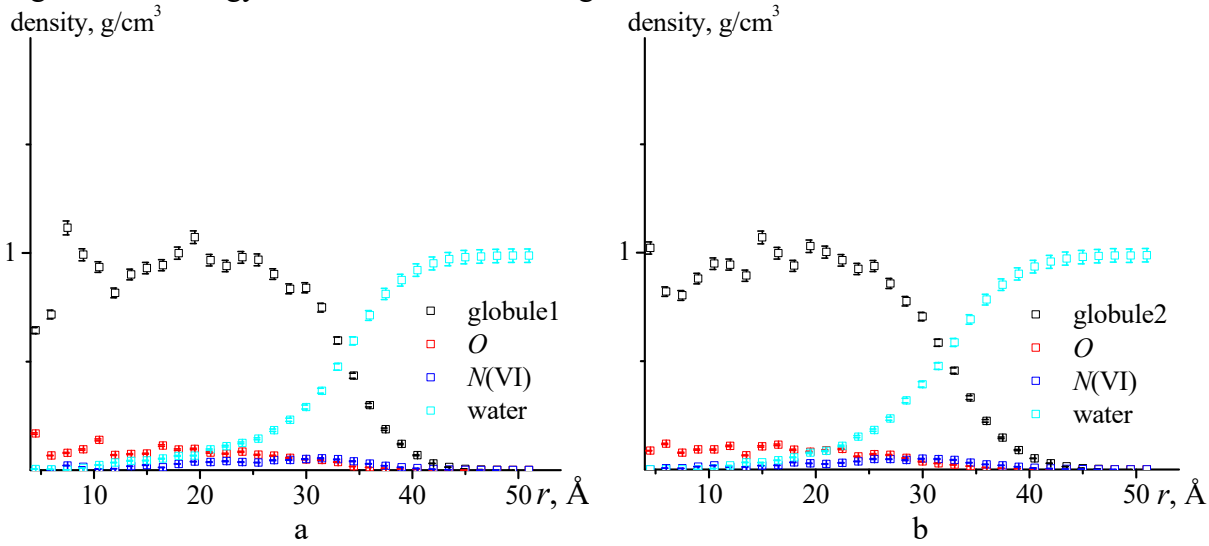

Fig. 3. Density distributions relative to the centers of mass of the «globule1» sample (a) and «globule2» sample (b). The black markers represent the total density of the globules, the red markers represent the oxygen atoms of VCL, the blue markers represent the nitrogen atoms in the VI ring (see Fig. 2), cyan markers represent the water molecules.

Fig. 3 shows the distribution of the atomic density relative to the center of mass of the globules. Both globules show similar patterns. The total density of the atoms is near constant within the body of the globule, and fluctuates only slightly. The distributions of atoms, specific to the VCL and VI units, namely, the oxygen atoms of the VCL and the nitrogen atoms of the VI ring, reveal a pronounced core-shell structure of the globules. The VCL units uniformly fill the core of the globules, and the VI units are located within the outer shell of the globules. One can also see that the water molecules penetrate the VI-rich shells of the globules, because the VI units have high affinity to water. At the same

time, within the VCL-rich cores the average densities of the water molecules quickly fall. This allows one to conclude that the bilayered core-shell structure of the model globules persists during the transition from the coarse-grained to the all-atom representation. At the same time, unlike the coarse-grained models, the all-atom ones considerably swell due to penetration of the water molecules.

Additionally, NP/water hydrogen bonds were calculated using the Hydrogen Bonds plugin in Visual Molecular Dynamics package [26]. For the first system, globule1, a value of 172 ± 11 was obtained, while for the second one, globule2, this value was equal to 162 ± 12, which is within the error range. The presence of a large number of hydrogen bonds between the globules and water molecules facilitates the formation of an ordered water layer around them. The presence of such a layer is an important factor preventing mutual aggregation of globules (precipitation).

4. Conclusion

An algorithm for converting the mesoscale globules of VCL-VI copolymers into all-atom representation was developed. The initial stability assessment was performed for two independent samples, corresponding to the synthesis parameters found most promising in the experimental research. The behavior of the studied models in an aqueous media allows concluding that the systems are stable. After the initial swelling, the radius of gyration of the globules is stabilized, indicating that the swelling stops. The globules revealed a pronounced core-shell structure, with the VCL monomer units forming the core and the VI monomer units forming the outer shell. The penetration of the water molecules into the globule roughly corresponds to the VI-rich shell. While the initial data suggests that the experimentally observed protein-like behavior of the copolymers can be explained by the morphology of the globules, the developed model will be used for an extensive study of the aggregation stability of the copolymer globules.

The work was carried out using equipment from the National Research Center 'Kurchatov Institute' (http://ckp.nrcki.ru/) and using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University [27]. Part of the data processing was performed at the Interlaboratory Computing Center of the Institute of Organoelement Compounds, A.N. Nesmeyanov of RAS, supported by the Ministry of Science and Higher Education of the Russian Federation.

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