

Dynamic Monte Carlo Simulation on Polymerization of Encapsulant

Chen Jin, Xiang Jiong-Hua

Cite this article as:

Chen Jin, Xiang Jiong-Hua. Dynamic Monte Carlo Simulation on Polymerization of Encapsulant[J]. *Chinese J. Polym. Sci.*, 2019, 37(2): 157-163. doi: 10.1007/s10118-019-2176-5

View online: <https://doi.org/10.1007/s10118-019-2176-5>

Articles you may be interested in

A COMPREHENSIVE MONTE CARLO SIMULATION OF STYRENE ATOM TRANSFER RADICAL POLYMERIZATION

Chinese J. Polym. Sci. 2010, 28(4): 483 <https://doi.org/10.1007/s10118-010-9058-1>

Monte Carlo Simulation on Layered Polymeric Films

Chinese J. Polym. Sci. 2014, 32(5): 595 <https://doi.org/10.1007/s10118-014-1446-5>

EXTENSIONAL FLOW OF BULK POLYMERS STUDIED BY DYNAMIC MONTE CARLO SIMULATIONS

Chinese J. Polym. Sci. 2013, 31(11): 1463 <https://doi.org/10.1007/s10118-013-1337-1>

高分子链坍塌转变动力学过程的动态蒙特卡罗模拟

DYNAMIC MONTE CARLO SIMULATION OF KINETIC PROCESS FOR POLYMER COLLAPSE TRANSITION

高分子学报. 2009(12): 1238 <https://doi.org/10.3724/SP.J.1105.2009.01238>

Monte Carlo 模拟预测汽油组分与聚酰亚胺相容性

PREDICTION OF MISCIBILITY OF POLYIMIDES AND GASOLINE COMPONENTS BY MONTE CARLO SIMULATION

高分子学报. 2012(4): 374 <https://doi.org/10.3724/SP.J.1105.2012.11193>

Monte Carlo 模拟方法研究管道受限对高分子链缠结的影响

MONTE CARLO STUDIES OF THE CONFINEMENT EFFECTS ON THE ENTANGLEMENT OF POLYMER CHAINS

高分子学报. 2011(5): 554 <https://doi.org/10.3724/SP.J.1105.2011.10134>

Dynamic Monte Carlo Simulation on Polymerization of Encapsulant

Jin Chen^{a*} and Jiong-Hua Xiang^b^a Department of Physics, Research Institute for Soft Matter and Biomimetics, Xiamen University, Xiamen 361005, China^b Department of Chemical Engineering, Shanghai Jiao Tong University, Shanghai 200240, China

Abstract Based on the preparative experiments of the light-emitting diode (LED) encapsulant, three types of monomer models with different functional groups are carried out to study the polymerization process by dynamic Monte Carlo (DMC) simulation and bond fluctuation model (BFM). We calculate the degree of polymerization, the radius of gyration and the frequency of void spheres to discuss the polymerization process, the molecular size and the spatial distribution at different volume fractions and proportions. Our results are in agreement with Grest's decay rate and Flory's scale law. Simulations show that the polymerization process depends on the appropriate volume fraction and proportion exceedingly, and the volume contraction in the polymerization process can also be observed in this study. These investigations could provide some insights into the understanding of the polymerization process of the encapsulant and help us to adjust the parameters in later experiments.

Keywords Dynamic Monte Carlo (DMC) simulation; Bond fluctuation model (BFM); LED encapsulant

Citation: Chen, J.; Xiang, J. H. Dynamic Monte Carlo simulation on polymerization of encapsulant. *Chinese J. Polym. Sci.* 2019, 37, 157–163.

INTRODUCTION

With the development of luminescent material and its preparation technology, light-emitting diode (LED) has a great potential to be the most effective solid-state lighting device for the requirement of energy-saving. It is currently under intense studies due to its promising traits that are not achievable with conventional light sources such as incandescent bulbs and fluorescent lamps. LED has the most outstanding features of high efficiency coupled with a long lifetime and the use of eco-friendly materials.^[1–4] In general, a LED lighting device is assembled with a LED chip packaged on a reflector cup with wires and heat sinks, which are all encased in an encapsulant with phosphors. The encapsulant plays a critical role in protecting the LED chip from external environmental conditions (such as water, oxygen, ultraviolet light or physical stress). A qualified LED encapsulant should have two basic features, a high refractive index for improving light transmission from LED chip and a sufficiently high thermal stability without yellowing during a long-term operation.^[5–7] The materials used for LED encapsulants are conventionally thermosetting epoxy resins, polyurethane resins, and silicone-based materials.^[8,9] Thermosetting epoxy resins generally have excellent optical transparency in the visible range and low gas permeability, but also have low refractive index. More importantly, they cannot maintain their transparency at the high operating temperature of LED and will undergo heat-induced yellow-

ing.^[10,11] Polyurethane resins can resist the heat, but it can be toxic to humans. To address this issue, silicone encapsulants are used as a LED encapsulant due to their excellent thermal stability and optical clarity.^[12] Many researchers are devoted to the research and development of high quality silicone encapsulants for diverse conditions.^[12–15]

Though there are many great achievements on the preparation of the encapsulant, the current theory can not explain the formation process and network structure of the encapsulant ideally. It is very difficult to understand the internal structure through experiments directly, whereas the molecular architecture of polymer networks strongly influences their physical and chemical behaviors. Therefore, computer simulation methods play an important role on solving this problem, and Monte Carlo (MC) simulation is exactly one of the effective methods and widely used for polymers.^[16–18] Although MC methods are usually employed to obtain the equilibrium properties of systems, they can also be used to study dynamical systems, and their use has been extended to the study of time-dependent properties.^[19–21]

Consequently, based on the discussion above, we build the monomer models to simulate the polymerization process in this research. These investigations may provide some insights into the understanding of the polymerization process of the encapsulant, which could help us to update the parameters in the next experiments.

MODEL AND METHOD

Model

The polymer chains are studied using the coarse-grained

* Corresponding author: E-mail chenjin@xmu.edu.cn

Received June 24, 2018; Accepted July 18, 2018; Published online August 3, 2018

bond fluctuation model (BFM) in three-dimensions on a simple cubic lattice,^[22–24] which has been widely used in recent years to investigate the structure and dynamics of a great variety of polymer systems.^[25,26]

The polymer is modeled as a self-avoiding walk on a lattice. Each bead in the model occupies a 2^3 cube of sites on a cubic lattice,^[27] and it is connected to another by a predetermined set of bond vectors. Next neighbors along the chain must be within a certain bond distance, so that the chain cannot cross itself. The bond vectors are built through all possible permutations and sign inversions of the following vector families:

$$\mathbf{B} = P(2,0,0)UP(2,1,0)UP(2,1,1)UP(3,0,0)UP(3,1,0)UP(2,2,1) \quad (1)$$

where $P(a,b,c)$ represents the set of all permutations and sign combinations of $(\pm a, \pm b, \pm c)$. The total number of possible configurations per bond is 108 as opposed to six for the simple cubic lattice; two consecutive bonds in BFM can take 87 different bond angles^[23] as opposed to two $(0^\circ, 90^\circ)$ for the simple cubic lattice. And note that the bond length between two consecutive beads can take five different values: 2, $\sqrt{5}$, $\sqrt{6}$, 3, and $\sqrt{10}$. Even though BFM is a lattice-based model, it does not suffer from the very discrete nature of the simple self-avoiding walk on a cubic lattice, whilst retaining the cheap overlap test characteristic of a lattice model. The set $\mathbf{B}$ is chosen to satisfy the constraints of both excluded volume between monomers and topological entanglement between chains. Only one monomer is permitted to occupy the same site and the entanglement constraint denies two chains to pass through each other for the excluded volume constraint.

Recently, phenyl-functionalized high refractive index silicone encapsulants have been reported.^[13–15] We also develop a kind of polysiloxane that can be used as LED encapsulant. In our experiments, methyl phenyl vinyl polysiloxane is synthesized by the hydrolysis and polycondensation reaction. The main raw materials are composed of phenyltrimethoxysilane, diphenyldimethoxysilane and 1,3-divinyltetramethyldisiloxane. Diphenyldimethoxysilane has two active functional groups, phenyltrimethoxysilane has three active functional groups, and 1,3-divinyltetramethyldisiloxane is the capping agent. According to our own preparation reaction, we set three initial monomer models (seen in Fig. 1), named type A, B, and C, respectively. One initial monomer model that has a star-shaped structure consists of five beads and four bonds. Type A has bifunctional groups, type B has trifunctional groups, and type C has monofunctional group.

The initial monomer models are placed in a cubic box under periodic boundary conditions at several volume fractions: $\varphi = 0.1, 0.2, 0.3, 0.4, 0.5$. The volume fraction of system is defined as:

$$\varphi = \frac{(N_a + N_b + N_c) \times 5 \times 2^3}{L \times L \times L} \quad (2)$$

where L is the length of cubic side, N_a , N_b and N_c is the number of type A, B and C monomers, respectively. We fix

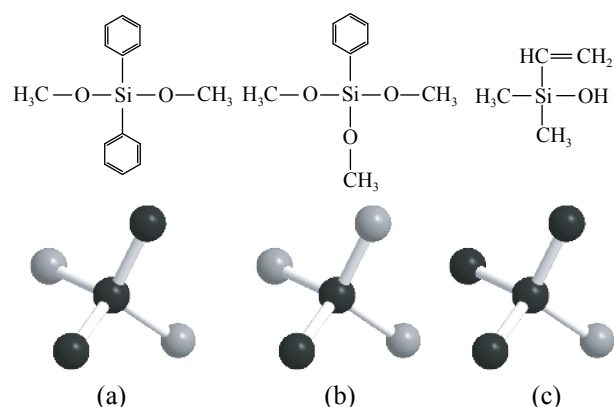


Fig. 1 Example diagrams of the monomer models: (a) bifunctional monomer, (b) trifunctional monomer, (c) monofunctional monomer (One gray bead represents one functional group.)

the cubic size with $L = 60$ and adjust the chain number to change the volume fraction or proportion in this research.

Method

The dynamic Monte Carlo method is widely used for modeling the dynamic behaviors of molecules, such as a reaction or diffusion.^[27,28] No matter polymerization occurs or not, the system should be first relaxed and self-diffuse under athermal conditions. In DMC simulation, only one type of move needs to be considered, namely the random jump of one bead in a randomly chosen lattice direction by single lattice spacing. The trial is accepted only if both the excluded volume and the bond length constraints remain unviolated. A Monte Carlo step (MCS) is defined as the number of successful attempts for each bead $5N_a + 5N_b + 5N_c$ to be chosen once on average. The snapshots of the relaxation process are illustrated in Fig. 2.

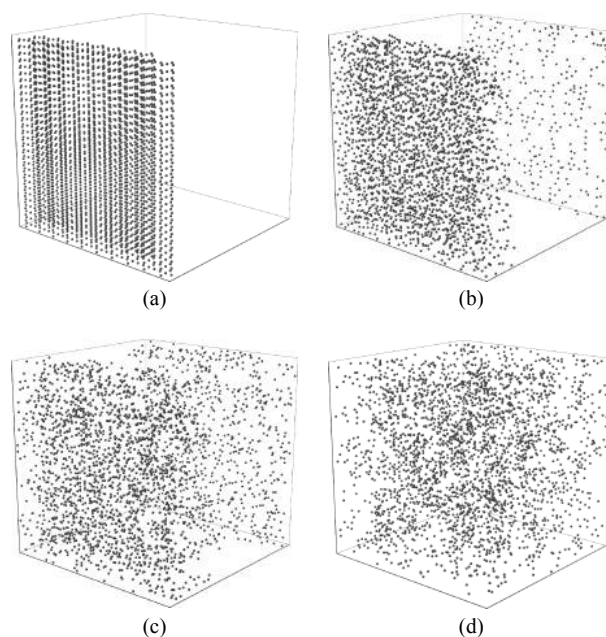


Fig. 2 Snapshots of relaxation process at $\varphi = 0.1$, a dot represents a monomer model (a) MCS = 0, (b) MCS = 50, (c) MCS = 500, (d) MCS = 5000.

After sufficient relaxation movements (MCS = 10000), an equilibrium state can be achieved as the initial states in the forthcoming simulation. We assume a polymerization reaction in this simulation, that a monomer could connect to another one by the interactions between two functional groups. In DMC simulation, when an unreacted bead is selected randomly, and it approaches another unreacted bead, a reaction always takes place between those beads, creating a new bond while it does not violate the excluded volume constraint and the allowed range of bond length either. But the reaction between two functional groups in the same monomer is not allowed here to avoid the ring structure. Furthermore, all kinds of systems evolve 100 times independently to count the ensemble average. Each evolutionary possesses 10000MCS, and the data are recorded per 200MCS.

RESULTS AND DISCUSSION

Polymerization Process

The focus of this study is on the differences in the evolution process at different volume fractions, varied from 0.1 to 0.5. To investigate the polymerization process of system growth, we calculate the fraction of unreacted beads from the new bonds formed as well as those at the end of reaction. The results with monomer proportion $N_a:N_b:N_c = 1:1:1$ are shown in Fig. 3. We find that the polymerization process, represented by slopes of decay, all proceeds fast as MCS increases. Grest *et al.* have suggested that the decay rate of the free beads in stoichiometric composition is extremely slow, with the power law behavior in time: $t^{-\alpha}$ with $\alpha \approx 0.5$.^[29] However, for a nonstoichiometric system, the decay is significantly faster.^[30] According to the kinetic interpretation based upon the master equation in statistics physics,^[31] the MC sampling process reflects the kinetics of the underlying physics, namely, the number of MCS is linearly proportional to the physical time. The results in Fig. 3 show the similar power law behavior. But the observed exponents are slightly higher than 0.5 at the larger volume fraction, which may be attributed to many short chains in this

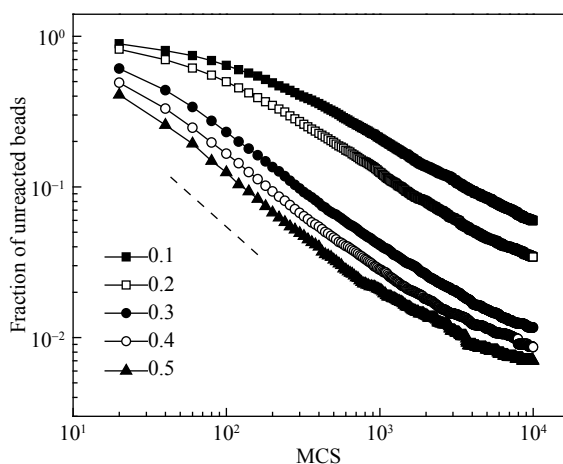


Fig. 3 Double logarithmic plots of the fraction of unreacted beads as a function of MCS at different volume fractions. The dash line is the slope of $\text{MCS}^{-\alpha}$ with $\alpha = 0.5$.

condition. Furthermore, in a certain volume, the probability of bonding could be higher with the number of monomers increasing, therefore the decay trend of the curves is more significant at larger volume fraction.

Fig. 4 shows the number-average degree of polymerization as a function of MCS at different volume fractions. The increase in the number-average degree of polymerization as the reaction progresses represents growth of polymer system directly, and this conclusion has been shown in Fig. 3 above. But we can find that there is a distinctive difference at large volume fraction in Fig. 4. In the case of $\varphi = 0.5$, the system form polymers more rapidly than all the others at the beginning of the reaction progresses, but when MCS is larger than 1000 approximately, the value of the curve with $\varphi = 0.5$ is smaller than the case of $\varphi = 0.3$. Similar result could be observed in the curves with $\varphi = 0.4$ and $\varphi = 0.3$ while the intersection appears in about MCS = 8000.

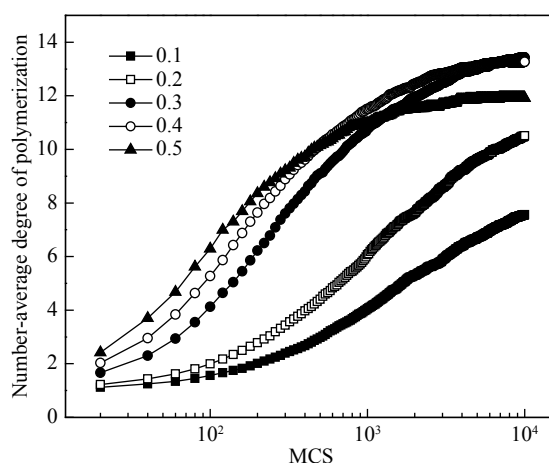


Fig. 4 Number-average degree of polymerization as a function of MCS at different volume fractions

In conclusion, the fundamental difference in polymerization progress is attributed to the volume fraction greatly. On the one hand, larger volume fraction means more initial monomers so that an unreacted functional group is more likely to meet another one. On the other hand, with the evolution processing, larger volume fraction blocks the diffusion of chains, which could slow down the polymerization reaction. Therefore, only an appropriate volume fraction can accelerate the polymerization progress in the specific experiments.

Molecular Size

As one of the basal parameters, root-mean-square radius of gyration under different conditions is shown in Figs. 5 and 6, respectively. The molecular sizes all increase with the polymerization process of systems, but the system with the large volume fraction grows rapidly in the initial polymerization stage while slowly in the late stage from Fig. 5. This result is consistent with the discussion in above section because of the diffusion of the chains.

According to the scaling theory of Flory,^[32] considering a dilute solution of polymer coil in a good solvent, the radius

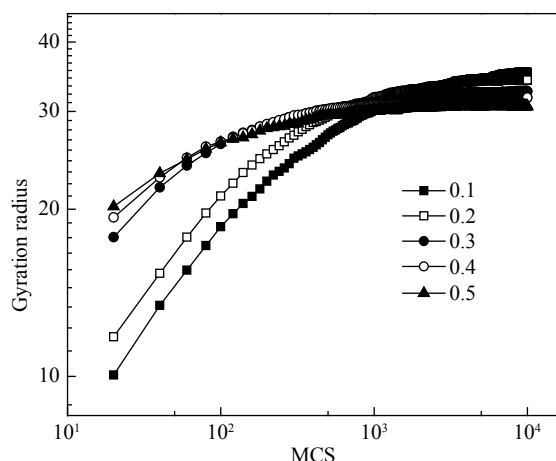


Fig. 5 Double logarithmic plots of the root-mean-square gyration radius as a function of MCS at different volume fractions

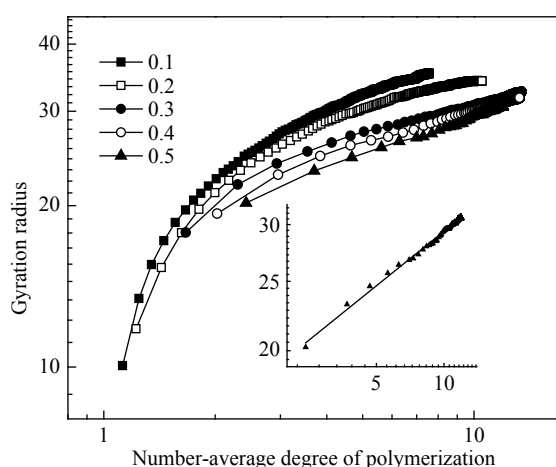


Fig. 6 Double logarithmic plots of the root-mean-square gyration radius as a function of the average degree of polymerization at different volume fractions. The small figure is the linear fitting for $\phi = 0.5$.

of gyration of one coil R_g depends on the degree of polymerization N , $R_g \propto N^\nu$. Similar results can be found in the late stage of polymerization from Fig. 6. At the initiation of polymerization reaction, there are many small monomers in the system and these monomers create the short coils firstly. With the evolution of polymerization reaction, these short coils form long polymer chains. We can find that in the late stage of polymerization, the double logarithmic plots of gyration radius and the average degree of polymerization obey the linear relation. Moreover, it is more obvious for the large volume fraction because the scaling law is better fit for the large number of chains. We fit the data ($\phi = 0.5$) to a linear line and add a small diagram to show this conclusion in Fig. 6.

Spatial Distribution

To study and evaluate a broad scale of the polymer network structure and its homogeneity, we use the void spatial distribution of the entire network to analyze its spatial homogeneity. A position is first selected randomly in the system as the center of sphere. The radius of the sphere is

gradually enlarged, keeping its center fixed, until the sphere contacts any beads. Once the sphere contacts any beads, the radius is saved, and this procedure is repeated over 10000 times. We calculate the average of spherical radius as a function of reaction time (MCS), and the result is shown in Fig. 7. We can get the conclusion that large volume fraction means more monomers and the corresponding spherical radius is small, which makes the system seems more ‘crowded’. And with the time increasing, the spherical spaces all increase slightly and synchronously at different conditions. Based on BFM, the bead movement must be subjected to the excluded volume and bond length constraint, when many ‘free’ functional groups are bound to the others with the ever-increasing bonds and the distances between the functional groups become shorter. In fact, most of the polymer systems will shrink in volume during polymerization. The main reason could be that the monomer molecules are originally tied to each other by van der Waals’ force but these interactions change to chemical bonds (covalent bonds) because of polymerization. It is obvious that the covalent bond distance is less than the van der Waals’ force distance, which leads to the volume contraction in the polymerization process inevitably.

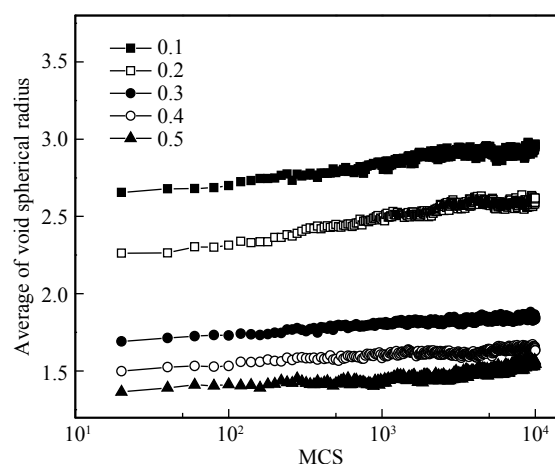


Fig. 7 Average of the void spherical radius as a function of MCS at different volume fractions

We also analyze the statistical dependence of the frequency of void sphere size on its radius, as shown in Fig. 8. Overall, the probability of too large or too small spheres is relatively low, and the radius is mainly concentrated near 2. The distributions of systems with large volume fraction have sharper peaks than those with small volume fraction, indicating that the systems with large volume fraction have spatially homogeneous network on a wide scale, while the systems with small volume fraction have large voids where a sphere of the same size could be placed. According to the normalization principle, curves with a smaller range have sharper peaks correspondingly, and these peaks will move to the small scale with the volume fraction increasing. We consider that when the number of initial monomers is small, the systems first form many small coils during the polymerization process simultaneously. These small coils grow radially

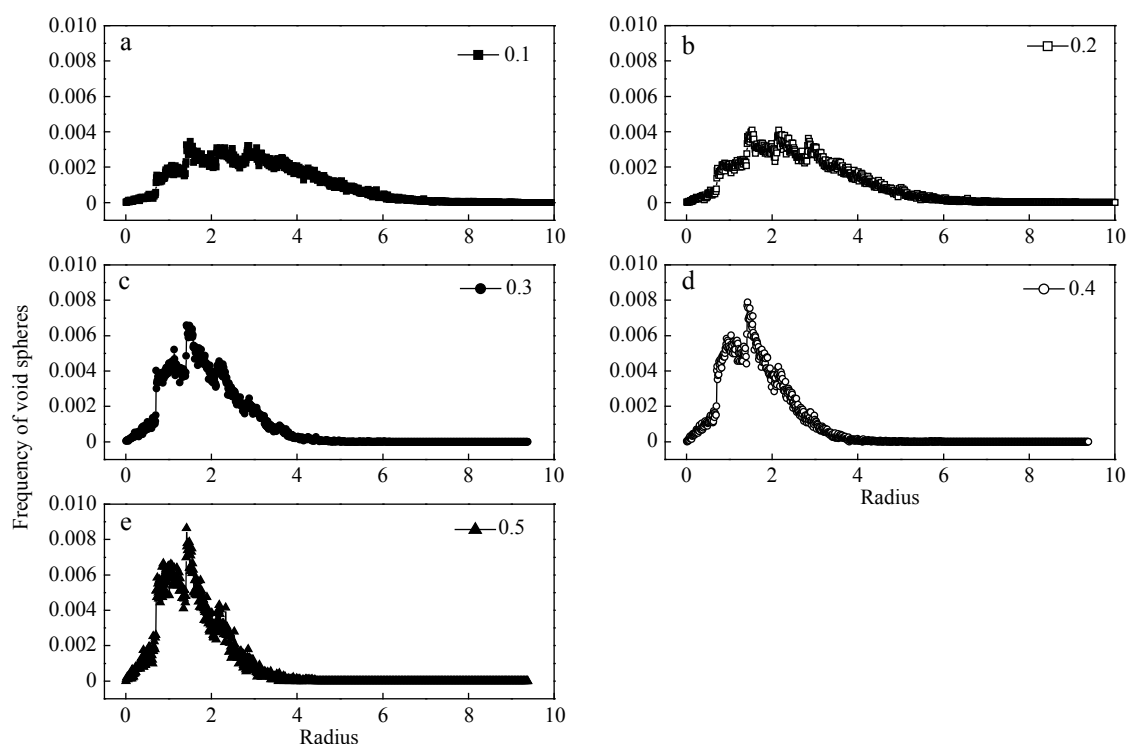


Fig. 8 Frequency of void sphere in the system (MCS = 10000) as a function of radius at different volume fractions (a) 0.1, (b) 0.2, (c) 0.3, (d) 0.4, (e) 0.5

with numerous initial monomers respectively and then take part in coil-coil aggregation to form complicated network structure when their sizes become large enough. At that point, the final network structures develop with large-scale inhomogeneity. When the number of the initial monomers is large enough, small coils transform into the network rapidly because of the excluded volume and the ‘stiff’ bond length constraints. We can get the conclusion that the systems at small volume fractions have the structures with many voids while the systems at large volume fractions form more homogeneous network with few voids. Furthermore, based on BFM, since the bond length is only divided into several discrete values, the frequency of the curves at larger volume fraction fluctuates more significantly.

Component Proportion

In practice, the polymers are required to possess various physical and chemical properties for multifarious condition. For example, the encapsulant must have high transmittance, high refractive index, good heat resistance, high thermal conductivity, high mechanical strength and chemical stability. And these properties are closely related to the network structure of the polymers. Thereupon, various proportions of the three initial monomers are listed here to form different structures. We select the system at the volume fraction 0.3, fix proportion of type A, and then change that of type B or C. The related curves with solid and hollow squares are drawn in Figs. 9 and 10. Similarly, the curves with circles and triangles represent the cases of fixed proportions of type B and C, respectively. As comparison, the results in above section ($N_a:N_b:N_c = 1:1:1 = 2:2:2$) are

also shown in the same figures with stars. It is meaningful that all data are almost overlapped in Fig. 9, which shows the polymerization process is seemingly independent of the proportions of three initial monomers. In contrast, there is a significant difference between the curves in Fig. 10. When the proportion of type B is high, the systems have lesser number of chains as can be found in the curves with hollow squares or triangles in Fig. 10. The reason may be that this type B have trifunctional beads, which tend to generate the radially complicated three-dimensional network system. But if we increase the proportion of type C, seen in the curves with solid squares or circles, the number of chains is larger

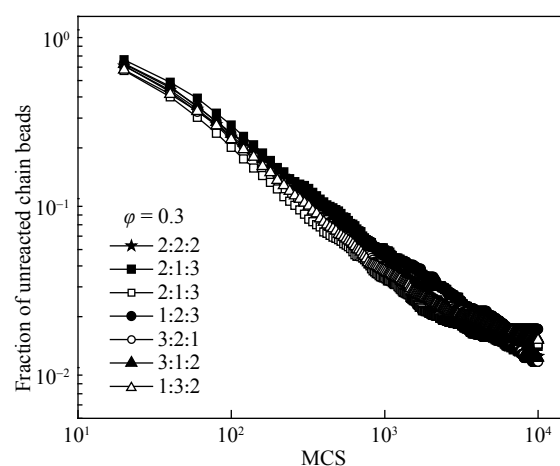


Fig. 9 Double logarithmic plots of the fraction of unreacted chain beads as a function of MCS at different proportions

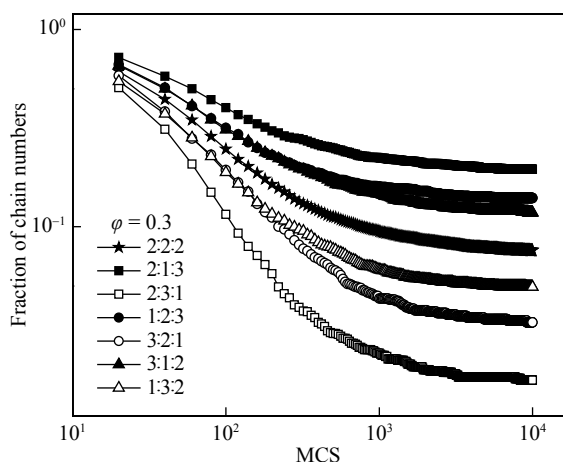


Fig. 10 Double logarithmic plots of the fraction of chains number as a function of MCS at different proportions

than the others. When any functional bead in type A or B is bonded to the functional beads in type C, the chain will stop growing and it leads to the formation of many short chains in the system. In the actual experiment, single functional group compounds are always added to eliminate the activity of end group, and type C monomers just act as the capping agents in our simulation. Overall, type B tends to construct a big crosslinking system while type C wants to stop this network growth. And type A connects to these two extremes, which can be added to generate more multifarious structures.

CONCLUSIONS

In this study, we use the dynamic Monte Carlo (DMC) simulation and bond fluctuation model (BFM) to discuss the polymerization process of three kinds of monomers with different functional groups. Our results are in agreement with Grest's decay rate $t^{-\alpha}$ and Flory's scale law $R_g \propto N^{\nu}$, which shows the method and the model are suited to the polymerization process. We calculate different parameters to study the influence of the volume fraction and the proportion for system structure. And the volume contraction in the polymerization process can also be observed in this simulation. These investigations could provide some insights into the understanding of the polymerization process of encapsulant and help us to adjust the volume fractions or proportions in the following experiments to produce diverse products for different operation circumstances. In addition, we will improve the system to bring it closer to the real polymer chain, and the mechanical and optical properties should be discussed to compare with the experimental data in the future.

REFERENCES

- Patel, P. Solid-state lighting: The future looks bright. *MRS Bull.* **2011**, *36*, 678–680.
- Tsami, A.; Yang, X. H.; Galbrecht, F.; Farrell, T.; Li, H.; Adamczyk, S.; Heiderhoff, R.; Balk, L. J.; Neher, D.; Holder, E. Random fluorene copolymers with on-chain quinoxaline acceptor units. *J. Polym. Sci., Part A: Polym. Chem.* **2007**, *45*, 4773–4785.
- Kanelidis, I.; Ren, Y.; Lesnyak, V.; Gasse, J. C.; Frahm, R.; Eychemüller, A.; Holder, E. Arylamino-functionalized fluorene- and carbazole-based copolymers: Color-tuning their CdTe nanocrystal composites from red to white. *J. Polym. Sci., Part A: Polym. Chem.* **2011**, *49*, 392–402.
- Tao, P.; Li, Y.; Siegel, R. W.; Schadler, L. S. Transparent dispensible high-refractive index ZrO_2 /epoxy nanocomposites for LED encapsulation. *J. Appl. Polym. Sci.* **2013**, *130*, 3785–3793.
- Narendran, N.; Gu, Y.; Freyssinier, J. P.; Yu, H.; Deng, L. Solid-state lighting: Failure analysis of white LEDs. *J. Cryst. Growth* **2004**, *268*, 449–456.
- Narendran, N.; Gu, Y. Life of LED-based white light sources. *J. Disp. Technol.* **2005**, *1*, 167–171.
- Chhajed, S.; Lee, W.; Cho, J.; Schubert, E. F.; Kim, J. K. Strong light extraction enhancement in GaInN light-emitting diodes by using self-organized nanoscale patterning of *p*-type GaN. *Appl. Phys. Lett.* **2011**, *98*, 071102.
- Hsu, C. W.; Ma, C. C. M.; Tan, C. S.; Li, H. T.; Huang, S. C.; Lee, T. M.; Tai, H. Effect of thermal aging on the optical, dynamic mechanical, and morphological properties of phenylmethylsiloxane-modified epoxy for use as an LED encapsulant. *Mater. Chem. Phys.* **2012**, *134*, 789–796.
- Huang, W.; Zhang, Y.; Yu, Y.; Yuan, Y. Studies on UV-stable silicone-epoxy resins. *J. Appl. Polym. Sci.* **2007**, *104*, 3954–3959.
- Bourget, L.; Corriu, R. J. P.; Leclercq, D.; Mutin, P. H.; Vioux, A. Non-hydrolytic sol-gel routes to silica. *J. Non-Cryst. Solids* **1998**, *242*, 81–91.
- Chung, P. T.; Yang, C. T.; Wang, S. H.; Chen, C. W.; Chiang, A. S. T.; Liu, C. Y. ZrO_2 /epoxy nanocomposite for LED encapsulation. *Mater. Chem. Phys.* **2012**, *136*, 868–876.
- Katayama, S.; Yamada, N.; Shibata, Y.; Noda, K. Fabrication and properties of PDMDPS-based inorganic/organic hybrid sheets. *J. Ceram. Soc. Japan* **2003**, *111*, 391.
- Mosley, D. W.; Khanarian, G.; Conner, D. M.; Thorsen, D. L.; Zhang, T.; Wills, M. High refractive index thermally stable phenoxypheyl and phenylthiophenyl silicones for light-emitting diode applications. *J. Appl. Polym. Sci.* **2014**, *131*, 39824.
- Kim, J. S.; Yang, S. C.; Kwak, S. Y.; Choi, Y.; Paik, K. W.; Bae, B. S. High performance encapsulant for light-emitting diodes (LEDs) by a sol-gel derived hydrogen siloxane hybrid. *J. Mater. Chem.* **2012**, *22*, 7954–7960.
- Kim, Y. H.; Bae, J. Y.; Jin, H.; Bae, B. S. Sol-gel derived transparent zirconium-phenyl siloxane hybrid for robust high refractive index LED encapsulant. *ACS Appl. Mater. Interfaces* **2014**, *6*, 3115–3121.
- Leach, A. R. in *Molecular modelling: principles and applications*. London, Longman, **2001**.
- Landau, D. P.; Binder, K. in *A guide to Monte Carlo simulations in statistical physics*. Cambridge, Cambridge University, **2000**.
- Newman, M. E. J.; Barkema, G. T. in *Monte Carlo methods in statistical physics*. Oxford, Clarendon Press, **2000**.
- Bortz, A. B.; Kalos, M. H.; Lebowitz, J. L. A new algorithm for Monte Carlo simulation of Ising spin systems. *J. Comput. Phys.* **1975**, *17*, 10–18.
- Gillespie, D. T. A general method for numerically simulating the stochastic time evolution of coupled chemical reactions. *J.*

- Comput. Phys.* **1976**, 22, 403–434.
- 21 Fichthorn, K. A.; Weinberg, W. H. Theoretical foundations of dynamical Monte Carlo simulations. *J. Chem. Phys.* **1991**, 95, 1090–1093.
- 22 Carmesin, I.; Kremer, K. The bond fluctuation method: A new effective algorithm for the dynamics of polymers in all spatial dimensions. *Macromolecules* **1988**, 21, 2819–2823.
- 23 Deutsch, H. P.; Binder, K. Interdiffusion and selfdiffusion in polymer mixtures: a Monte Carlo study. *J. Chem. Phys.* **1991**, 94, 2294–2304.
- 24 Paul, W.; Binder, K.; Heermann, D. W.; Kremer, K. Crossover scaling in semidilute polymer solutions: A Monte Carlo test. *J. Phys. II* **1991**, 1, 37–60.
- 25 Wittkop, M.; Kreitmeier, S.; Goritz, D. The collapse transition of a single polymer chain in two and three dimensions: A Monte Carlo study. *J. Chem. Phys.* **1996**, 104, 3373–3385.
- 26 Wilding, N. B.; Muller, M.; Binder, K. Chain length dependence of the polymer-solvent critical point parameters. *J. Chem. Phys.* **1996**, 105, 802–809.
- 27 Shu, R. F.; Zha, L. Y.; Eman, A. A.; Hu, W. B. Fibril crystal growth in diblock copolymer solutions studied by dynamic Monte Carlo simulations. *J. Phys. Chem. B* **2015**, 119, 5926–5932.
- 28 Dasmahapatra, A. K.. Effect of composition asymmetry on the phase separation and crystallization in double crystalline binary polymer blends: A dynamic Monte Carlo simulation study. *J. Phys. Chem. B* **2017**, 121, 5853–5866.
- 29 Chen, C. M.; Higgs, P. G. Monte-Carlo simulations of polymer crystallization in dilute solution. *J. Chem. Phys.* **1998**, 108, 4305–4314.
- 30 Grest, G. S.; Kremer, K.; Duering, E. R. Kinetics of end cross-linking in dense polymer melts. *Europhys. Lett.* **1992**, 19, 195.
- 31 Binder, K.; Heermann, D. W. in *Monte Carlo simulation in statistical physics: An introduction*. 3rd ed.; Springer-Verlag, Berlin, **1997**.
- 32 De Gennes, P. G. in *Scaling concept in polymer physics*. Cornell University Press, **1979**.