Application of Computer Simulation in Packaging Material

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Abstract: As an important packaging material, the property of size, shape and solubility etc. of polymer material attracts more and more widespread attention. In polymer solution, the size, shape and solubility of the polymer chain has an affinity with the interaction energy between the solvent molecules and the chain molecules. Besides the experiment measure, the numerical value investigation of the model chain is a very important method to study polymer. Monte Carlo (MC, computer simulation) method was a particular research method situated between theory and experience methods. The application of computer simulation was realized with the simulation on the size, shape and solubility of the packaging polymer material. The author attempts to adopt Monte Carlo compute method of calculating the changing energy value directly fore-and-aft movement to simulate the linear polymer and makes a research on the variational situation of polymer property with the interaction energy changing among the system components.

Keywords: packaging material; computer simulation; property

1. Introduction

Solubility of the polymer has attracted much attention for their being one of core problems of the polymer physics. Besides the experiment measure, the numerical value investigation of the model chain is a very important method to study polymer. Monte Carlo (MC, computer simulation) method was a particular research method situated between theory and experience methods. Numerical methods that are known as Monte Carlo methods can be loosely described as statistical simulation methods, where statistical simulation is defined in quite general terms to be any method that utilizes sequences of random numbers to perform the simulation. Xiaozhen Yang [1], Delu Zhao and Yuliang Yang [2] etc determine the energy of the system and discuss the solubility by confirming the number of the interaction pairs. Our work is to attempt to adopt Monte Carlo compute method of calculating the changing energy value directly fore-and-aft movement to simulate the linear polymer multiple chain systems lattice model, and makes a research on the variational situation of polymer solubility with the interaction energy changing among the system components.

2. Model and Compute Method

We study the polymer multiple chains model and build simple cube lattice SAW chain using dynamic MC. The method of generating the sample is giving birth to the new configuration by movement of the polymer chain. For the polymer multiple chains system, the volume fraction Φ is

$$\Phi = cn \times n / L^3 \tag{1}$$

Where *cn* is the numbers of the polymer chain, *n* is the chain length, *L* is the length of the simple cube lattice model.

Different from the method many people have used that determine the energy by the number of the interaction pair of the molecule chain, the author adopts a new compute energy measure to process the simulation attempt. We account the energy change value of the movement chain segment before moving and after moving respectively (before moving, count the energy value between the chain segment (A) that demand movement together with the empty site (B) that demand accept the movement chain segment and the circumference molecule; after moving, count the energy value between the chain segment (A') after movement together with the generated empty site (B') and the circumference molecule). Using this means can deal with the diverse energy respectively, we can study the effect of the change of the energy in system on the linear polymer chain model more exactly. On account of considering the interaction, diverse chain conformation possess different energy, we also apply Metropolis algorithm to generate the new conformation in effect, the incept probability of the new conformation P

$$P = \begin{cases} 1, & \Delta E \le 0 \\ e^{-\Delta E / kT}, & \Delta E > 0 \end{cases} \tag{2}$$

ΔE is the energy difference. *E*ss, *E*pp and *E*ps are the interaction energy for solvent molecule-solvent molecule, polymer chain segment-polymer chain segment and solvent molecule-polymer chain segment at near neighbor position. We use relevance parameter $\varepsilon_{SS} = Ess / kT$, $\varepsilon_{PP} = Epp / kT$ and $\varepsilon_{PS} = Eps / kT$ to denote the size of the interaction energy, where *k* is Boltzmann constant, the absolute temperature *T* is a constant value. The relevance energy unit size is $\varepsilon(\varepsilon>0)$, the repulsion energy is ε,

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the attraction energy is $-\varepsilon$ [3].

We simulate the linear polymer chain lattice model in the energy condition of $\varepsilon_{SS}=-\varepsilon$, $\varepsilon_{PP}=-\varepsilon$ and ε_{PS} between -2ε and 2ε. As well as we discuss polymer solubility in the condition that the chain length n=20, 50, 100 when the volume fraction $\Phi=0.125$.

3. Results and Discussion

We set the needed concentration polymer chains in the simple cube lattice evenly just as Fig. 1 showing. In the course of the simulation, we note the required parameter value in the simulation time intervals and observe that the discrepancy of the parameter value is not too big when we generate 100,000 samples to obtain the mean value, so we can think it has already constringed, just as Fig. 2 showing. Therefore we figure that the adopted simulation values in this article are in reason.

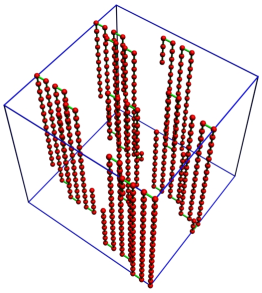

Figure 1. Original typical configurations of the multiple chain systems for the n=50.

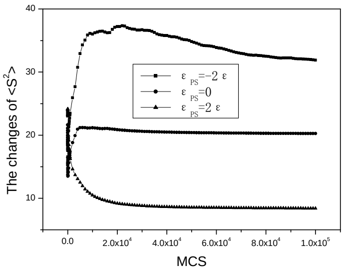

Figure 2. The changes of $<S^2>$ with variation of MCS for the n=100 when the volume fraction Φ=0.125.

People find that the polymer chain is the ruleless coil shape from the experiment. The size of the coil is stretched in good solvent and shrinked in bad solvent. For a polymer chain, increase of the close contact means that the contraction of coiled molecule, not conducive to stability in the solvent. Therefore, the total number of the nearest interaction pairs can be used to express the solubility of the good or bad.

We study the changes of the nearest interaction pairs among the same polymer chain segment molecule, the nearest interaction pairs among the different polymer chain segment molecule, the total nearest interaction pairs among the polymer chain segment molecule and the nearest interaction pairs between the solvent molecule and the polymer chain segment molecule with variation of the interaction energy ε_{PS} respectively. Fig. 3 and Fig. 4 shows increase of the nearest interaction pairs among the same polymer chain segment molecule and the nearest interaction pairs among the different polymer chain segment molecule with increase of ε_{PS} means chain monomer units are more uniform distribution in the solvent when attraction between the solvent molecule and the polymer chain segment molecule is stronger. With increase of ε_{PS}, polymer chains arrange intensively locally, shrink and overlap across. At the volume fraction Φ=0.125, when repulsion between the solvent molecule and the polymer chain segment molecule is stronger, decrease of the nearest interaction pairs among the different polymer chain segment molecule means the intramolecular contraction is main mode for the reason of the system we investigated is not high density system.

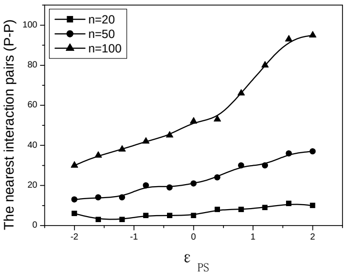

Figure 3. The changes of the nearest interaction pairs among the same polymer chain segment molecule with variation of the interaction energy ε_{PS}.

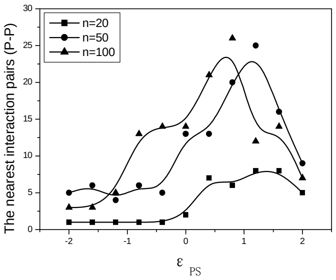

Figure 4. The changes of the nearest interaction pairs among the different polymer chain segment molecule with variation of the interaction energy ε_{PS}.

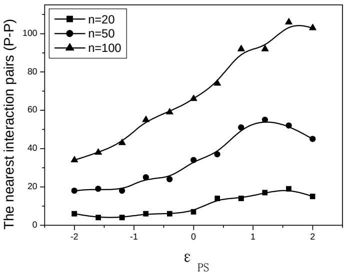

Figure 5. The changes of the total nearest interaction pairs among the polymer chain segment molecule with variation of the interaction energy ε_{PS}.

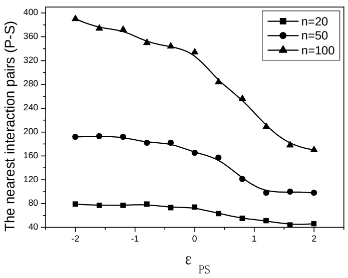

Figure 6. The changes of the nearest interaction pairs between the solvent molecule and the polymer chain segment molecule with variation of the interaction energy ε_{PS}.

Fig. 5 and Fig. 6 shows increase of the total nearest interaction pairs among the polymer chain segment molecule (include the nearest interaction pairs among the same polymer chain segment molecule and the nearest interaction pairs among the different polymer chain segment molecule) and yet decrease of the nearest interaction pairs between the solvent molecule and the polymer chain segment molecule with increase of ε_{PS} means contraction of the polymer chain and decline of solubility.

Therefore the value $\Delta\varepsilon$ determine the quality of the solvent, when polymer chain in good solvent, the solubility of the polymer chain is preferable, with the increase of the $\Delta\varepsilon$, the solvent become not benefit to solve, through to the polymer separate out as the deposition. From Fig. 7 to Fig. 12 show Typical configurations of the polymer chain for n=20, 50 and 100 when ε_{PS}=-2ε and ε_{PS}=2ε.

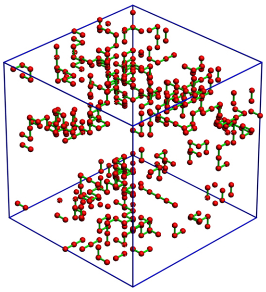

Figure 7. Typical configurations of the polymer chain for the n=20 when ε_{PS}=-2ε.

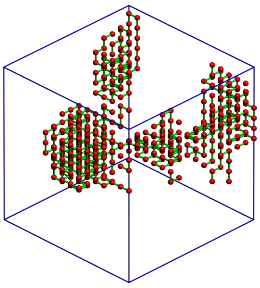

Figure 8. Typical configurations of the polymer chain for the n=20 when ε_{PS}=2ε.

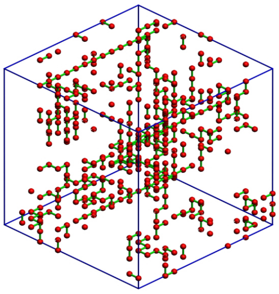

Figure 9. Typical configurations of the polymer chain for the n=50 when ε_{PS}=-2ε.

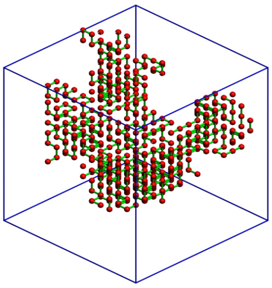

Figure 10. Typical configurations of the polymer chain for the n=50 when ε_{PS}=2ε.

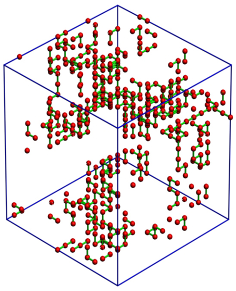

Figure 11. Typical configurations of the polymer chain for the n=100 when ε_{PS}=-2ε.

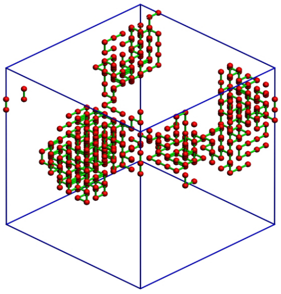

Figure 12. Typical configurations of the polymer chain for the n=100 when ε_{PS}=2ε.

4. Conclusion

From the simulation data, we can see that the method is an effective and original means to simulate the linear polymer multiple chain systems solubility. The results indicate, the solvent become not benefit to solve, the polymer chain turn into the ruleless coil shape, and the polymer groups overlap across with the increase of the interaction energy ε_{PS} between solvent molecule and polymer chain segment molecule.

5. Acknowledgment

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References

[1] Jiao X S; Zhao D L; Yang X Z. “Monte Carlo simulation of the polymer single-chain thermodynamic quantity,” Science in China(Series B), vol. 27, pp. 522-524, December 1997.

[2] Xu G Q; Zhu J X; Ding J D; Yang Y L. “Monte Carlo simulation of phase separation kinetics in a concentrated polymer solution,” Science in China(Series B), vol. 28, pp. 309-311, August 1998.

[3] Zhang Q L; Han Z R; Liu F Q. “Monte Carlo Simulation on Dynamic Behavior of Polymer Chains,” Journal of Jilin University (Science Edition), vol. 44, pp. 113-117, January 2006.