# A Difference in the Molecular Dynamics between the model Glass and Crystal

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I have computed a series of the molecular dynmics simulation for a model molecule. A molecule has 20 united atoms and the system has 2,000 molecules in the rigid cube with about 1,000 nm$^3$ volume and the periodic boundary condition. The molecules have the bonds between the united atoms nearby, the bends to the next bond, and the torsional potential. The DREIDING [1] potential parameters have been used in this research. Two different initial configurations represent "i3" and "i5" at temperature 700K. Two different cooling methods represent "str" and "st2" from 700K to 300K. The str and st2 means straightly and stepwisely cooled, each other. I have gained 50,000 configurations which elasping 0.2 pico second in the NVE ensemble for each sample.

Table 1: The distance dependence of the global orientational order parameters for the four samples.

| distance [nm] | i3str | i5str | i3st2 | i5st2 |
|---|---|---|---|---|
| 1.0 | 0.64 | 0.63 | 0.80 | 0.87 |
| 2.0 | 0.35 | 0.35 | 0.65 | 0.83 |
| 3.0 | 0.09 | 0.11 | 0.44 | 0.79 |
| 5.0 | -0.02 | -0.01 | 0.28 | 0.79 |

The global orientational order parameters are represented in the Table 1 for the four samples.

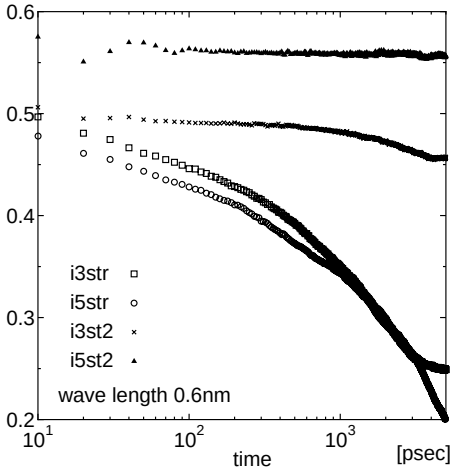


Figure 1: The density autocorrelation function in long time. The symboles square, circle, cross and triangle mean the samples of i3str, i5str, i3st2 and i5st2 respectively.

Only one sample i5st2 seems crystal, the orientational order extends to the whole system. The samples i3str and i5str seem glasses but with some micro-crystals. The sample i3st2 seems to have the middle character of these.

The dynamical character is shown in Figure 1. The density autocorrelation function in long time over 100 pico second is different between glass and crystal. The long time relaxation remains in glasses.

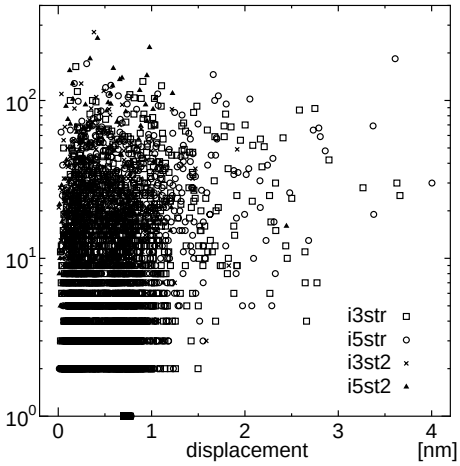


Figure 2: The displacements of the diffusion of each molecule for whole simulation time versus the counts of the jump motions for each molecule.

The source of this difference is the motion of molecules. The displacements of the diffusion of each molecule for whole simulation time versus the counts of a motion for each molecule is shown in Figure 2. A motion called "jump motion" has defined the motion which moves 0.7nm in 10psec. The molecule has about 2.3nm length, so 0.7nm is very large.

The displacements of some molecules in glass move over 2nm, but in crystal that are limited in 2nm. The str sample has about twice number of jump motions from the st2 sample. But I think the number is less important than the character of jump motion. I will show you the difference in the molecular dynamics between the model glass and crystal.

## References

[1] S. L. Mayo, B. D. Olafson, and W. A. Goddard III, J. Phys. Chem. **94**, 8897 (1990).