APPENDICES

APPENDIX A
THESIS OUTPUT (PUBLICATIONS)

1. **Kusinram, C.** and Vao-soongnern, V. (2024). Monte Carlo simulation for the effect of chain stiffness on the free surface of polymer melts. *Journal of Molecular Liquids*, *411*, 125665.
2. **Kusinram, C.** and Vao-soongnern, V. (2025). Monte Carlo simulation for the role of intermolecular interaction on polymer crystallization from the melts. *Journal of Molecular Liquids*, *418*, 126733.

APPENDIX B

INTERNATIONAL CONFERENCE I

The 17th International Workshop for East Asian Young Rheologists (IWEAYR-17), Busan, Korea.

The 16th International Workshop for East Asian Young Rheologists Conference
IWEAYR-16, Udon Thani, Thailand, Feb 18-21, 2023

P39

Multiscale Molecular Simulation of Structures and Dynamics Poly(vinyl chloride) Blends with Different Stereochemical Sequences

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Abstract

A multiscale simulation of amorphous polymeric materials has been developed for vinyl polymer with polar atoms *i.e.* polyvinylchloride, (PVC), -[CH2-CH(Cl)]n melts and binary blends with different chain tacticity (iPVC, sPVC and aPVC) at the bulk density. The model starts from an *ab initio* quantum chemistry to get the statistical weights of the rotational isomeric state (RIS) model to describe the conformational characteristics of polymer molecule. PVCs chains were coarse-grained by grouping one monomer in one bead and then mapped onto the second nearest neighbor diamond (*2nnd*) lattice. The average non-bonded interactions were treated by the discretized Lennard-Jones (LJ) potential. The on-lattice properties can be determined including chain dimension, intermolecular packing, conformational statistics and molecular mobility (rotational and translational modes). Dynamics of PVC chains with different stereochemistry were generally in the order as: iPVC > aPVC >> sPVC. For binary mixtures composed of chains with different stereochemical sequences, sPVC melt has a tendency for the formation of "local structure" than other types. The binary mixtures containing sPVC experience demixing during the simulations. Fully atomistic amorphous PVC models can be obtained by the reverse-mapping procedure to restore the missing atoms. After energy minimization, material properties including torsional angle distribution, solubility parameter, radial distribution function and static neutron scattering structure factor were calculated for neat structures and blends with different tacticity.

Keywords: Poly(vinyl chloride), Tacticity, Multiscale molecular simulation

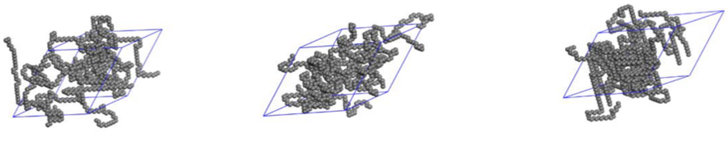

Fig. 1 Specific snapshots of (a) isotactic (b) atactic and (c) syndiotactic PVC models

Fig. 2 (a) The pair correlation function (chain packing) of *i*PS chains in pure melt and blend mixtures. (b) the mean-square displacement of the center-of-mass (MSD) of *i*PVC chains in pure melts and *i*PVC/*s*PVC, *i*PVC/*a*PVC blends.

References

1. V. A Multiscale Simulation Model for Poly(ethylene oxide), Polym., Sci. A, 2014, 56(6), 928.

APPENDIX C

INTERNATIONAL CONFERENCE I

International Discussion Meeting on Polymer Crystallization (IDMPC 2024), Yonezawa, Yamagata, Japan.

P1-30

Molecular simulation for the effect of interchain interaction on polymer crystallization upon step-wise cooling from the melts

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Monte Carlo (MC) simulation of coarse-grained models on the high coordination lattice was employed to investigate the effect of interchain interaction on the structural formation of "*polyethylene-like*" model upon stepwise cooling from the melt states. Polymer chains were represented by the Rotational Isomeric State model for intrachain energetics of polyethylene (*PE*) whereas the Lennard-Jones potential function for the interchain interactions ($\sigma = 0.44$ nm, $\varepsilon/k = 185$ K) for PE; ($\sigma > 0.44$ nm, $\varepsilon/k < 185$) or ($\sigma < 0.44$ nm, $\varepsilon/k > 185$) for polymer chains more repulsion or more attraction than that of normal PE, respectively). The evolution of the ordered structure was analyzed regarding the fraction of *trans* state, the length of *trans* sequence, the orientational order parameter at bond and molecular scale, the intermolecular pair correlation function, and the anisotropic change of chain dimension. Simulation results indicate that the rate of structural formation is faster and the degree of crystallinity is higher for normal PE chains. Chains with too strong attractive or too repulsive interaction adopt less amount of *trans* conformation and are harder to form the ordered structure upon cooling from the melts. Our study implies that only polymers with the appropriate range of interchain interaction can exhibit clear evidence for crystallization. [1-4].

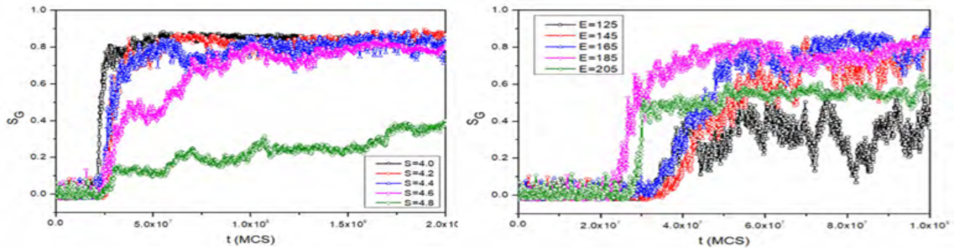

Figure 1 The evolution of the overall orientation correlation function for *polyethylene-like* models with different interchain interaction [left: varied σ and right: varied ε/k].

References
[1] S. Jamornsuriya and V. Vao-soongnern, J. Mol. Liq. **363**, 119833 (2023).
[2] V. Vao-soongnern, N. Sukhonthamethira, K. Rueansri, K. Sirirak, G. Matsuba, J. Mol. Liq. **376**, 121434 (2023)
[3] K. Rueansri and V. Vao-soongnern, J. Mol. Liq. **390**, 123134 (2023).
[4] K. Rueansri and V. Vao-soongnern, Macromol. **Symp. 409**, 2200146 (2023).