

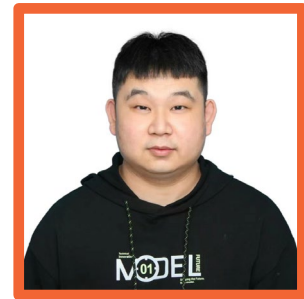
# Graduate Student Research Seminar

## Spring 2024

### Revealing the Effect of Nanoconfinement on the Crystallization Process of Semicrystalline Polymers Using Coarse-Grained Molecular Dynamics Simulations

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**Advisor: Dr. Zhaoxu Meng**

**Monday, April 15<sup>th</sup>**  
**3:00 pm (EST) – 132 Fluor Daniel Building**



#### Abstract

Semicrystalline polymers under nanoconfinement show distinct structural and thermomechanical properties compared to their bulk counterparts. Despite extensive research on semicrystalline polymers under nanoconfinement, the nanoconfinement effect on the crystallization process and the unique structural evolution of such polymers has not been fully understood. In this study, we aim to understand such effect by using coarse-grained molecular dynamics simulations to study the crystallization process of a model semicrystalline polymer - polyvinyl alcohol (PVA) - under different levels of nanoconfinement. We quantify the evolution of the degree of crystallinity ( $X_C$ ) of PVA and examine distinct crystalline regions from simulation results with great detail. The results indicate that nanoconfinement can promote the crystallization process, especially at the early stage, and the interfaces can function as crystallite nucleation sites. In general, final  $X_C$  of PVA increases with the level of nanoconfinement. Further, nanoconfined cases show region-dependent  $X_C$  within PVA, with higher  $X_C$  in regions closer to interfaces, i.e., nanoconfinement origins. By tracking region-dependent  $X_C$  evolution, our results indicate that nanoconfinement can lead to a heterogenous nucleation process with second-stage crystallite nucleation in regions further away from nanoconfinement origins. In addition, the results show that even with the highest cooling rate, the nanoconfinement still promotes the crystallization of PVA. This study provides insights into the underlying mechanisms for the intricate interplay between nanoconfinement and the crystallization behavior of semicrystalline polymer, with the potential to guide the design and characterization of semicrystalline polymer-based nanocomposites.



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