

Abstract Submitted  
for the APR20 Meeting of  
The American Physical Society

**Nucleation and Phase Transition in Block Copolymers**<sup>1</sup> PING TANG<sup>2</sup>, JINGYU SHAO, Fudan University — We combine the self-consistent field theory (SCFT) and the string method to explore the phase transition pathway and the critical nucleus information of rod-coil block copolymers. It is the first time to predict the size, shape and the energy barrier of the critical nucleus with segment orientation in the order-order phase transition path of rod-coil block copolymers. We observe significant differences in nucleation transition process between different orientations of  $\langle 111 \rangle$  cylinders and (101) lamellae. If the overall orientation of the initial cylinders is consistent with the object lamellae, the critical nucleus will have smoother surface and lower energy barrier. In contrast, rod blocks undergo multiple rearrangement orientations, and the nucleation progress is more difficult with higher nucleation energy barrier. This work has important guidance to the nucleation behavior and nucleating agent design in the phase transition process especially for polymer crystallization.

<sup>1</sup>National Natural Science Foundation of China. 21973017, 21774027

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Date submitted: 17 Jan 2020

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