Nucleation Study for Methane Hydrate by Molecular Dynamics

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Clathrate hydrate are solid crystalline compounds most commonly formed from solution to nucleate a mixed solid composed of water and gas. Understanding the mechanism of clathrate hydrate nucleation is crucial for a fundamental study of formation of these complex structures and their applications. Molecular Dynamics (MD) simulation is an ideal method to observe nucleation at the molecular level because the size of the critical nucleus and the nucleation time are nano scales. Various analysis methods have been developed through MD simulations to analyze nucleation in monatomic systems.[1,2] In particular, the nucleation rate, the critical nucleus size, and the free energy curve can be obtained from mean first-passage time, survival probability, and Yasuoka-Matsumoto methods. However, clathrate hydrate nucleation is difficult to observe in MD simulations due to high free energy barriers, so these methods have not been applied to clathrate hydrate systems. Recently, methane hydrate nucleation has been observed by MD simulations at 255 K and 50 MPa using high performance computing.[3] In this study, we analyzed methane hydrate nucleation using these methods for data generated from MD simulations and verified the applicability of these methods for the methane hydrate nucleation analysis. These methods are also easily applicable to other complex clathrate hydrate structures.

References

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