PB 15

Molecular dynamics study on nucleation process for supersaturated ZnO solutions in hydrothermal conditions

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Key Word (3 words)

Hydrothermal, Molecular simulation, Nucleation

Abstract (less than 300 words)

Molecular dynamics simulations were performed to investigate homogeneous nucleation mechanism of zinc oxide in ambient and hydrothermal conditions. Water model used in this work was the three-site flexible-SPC model proposed by Honma [1]. Atomic models for zinc and oxygen ions were constructed with Lennard-Jones and Coulomb potentials. The snapshot analysis of zinc oxide aqueous solution showed the two-step nucleation process, in which ions and water aggregate to form disordered clusters, followed by the crystallization of ions and solvent ejection. In case of ambient condition, the nucleation process of aqueous zinc oxide solution should be followed the two-step process, however, our simulation could not simulate the crystallization process as latter step due to slow nucleation process.

Radial distribution function of Zn^{2+} - O^{2-} revealed crystallization occurred at high zinc oxide concentration (N_{ion}=40), because sharp first and second peaks of g(r) were observed in all temperature conditions. This trend was more significant at high temperature conditions. In case of low zinc oxide concentrations (N_{ion}=5), the broad peak on g(r) were located around 6 Å up to 333 K. Zn^{2+} and O^{2-} ions would be solvated and moved independently. However, as increasing temperature, first peak of g(r) at low zinc oxide concentrations observed shorter and higher. This trend indicates nucleation rates at hydrothermal condition was faster than rates at ambient conditions. Therefore, the molecular dynamics simulation would be represented the difference of nucleation rate in temperature, and it may be determined the nucleation rate and critical nucleus size. The critical nucleus size and free energy analysis is in progress, which will be discussed in the presentation.

References:

[1] T. Honma, S. Kuzuhara, C.C. Liew, H. Inomata, Phase behavior and physico-chemical properties of aqueous electrolyte solutions near the critical point via molecular dynamics simulation with gravity perturbation, Fluid Phase Equilibria, 194-197 (2002) 271-280.

MTMS '21