Theoretical Analysis of Crystallization through Homogeneous Nucleation in Water Droplets

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The crystallization process of water droplets is of great practical and fundamental importance in science and technology. So far, many experiments of homogeneous ice nucleation of water droplets were performed. We propose a theoretical model describing nucleation of crystallization from supercooled water droplets based on nucleation theory, where we solve the time evolutions of homogeneous ice nucleation and the crystal growth in the cooling. With this model, we obtained the crystallization temperature and the number of the crystal nuclei. In the case that the particle size is from 1 micron to 1 mm, the crystallization temperature is 230- 240K for the cooling rate less than $10^4 Ks^{-1}$. If the cooling rate is beyond $10^4 Ks^{-1}$, the crystallization temperature decreases rapidly. On the other hand, in the case that the particle size is 10 nm, the crystallization temperature is 200-230K for the cooling rate less than $10^4 Ks^{-1}$. The analyses explain very well the crystallization temperatures obtained in the previous experiments including the crystallizations of nano-size to mm droplets with various cooling conditions. Our model also enables us to evaluate the critical value of cooling rate for vitrification of liquid water droplets. The results suggest the critical cooling rate for vitrification as well as the crystallization temperatures of water droplets depends on the droplet size. The comprehensives analysis for many experiments would be valuable not only for understanding of the ice nucleations of droplets, but also the prediction of crystallization process in the various environments.

Keywords: nucleation, crystal growth, water, supercooled water

