Bifurcation and Metastable States in Phase Transitions of Nucleotide Hydrates

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The understanding of phase transitions of molecular crystals is important from the view points of solid-state chemistry and material sciences. We have been investigating the first-order phase transitions of nucleoside and nucleotide hydrates [1]. Conformational changes and shifts of molecular layers were observed coupled with increase or decrease of crystal water molecules. In addition, the transitions are characterized by hysteresis and emergence of metastable states.

One typical example is the transition of disodium 2´-deoxyguanosine 5´-phosphate (Na_2dGMP) between the tetrahydrate and the anhydrous forms. Besides hysteresis, bifurcation of phase transition was observed. The tetrahydrate transforms to two different anhydrous forms, A and B. The ratio depends on the transition temperature which is correlated to vapor pressure of water. In the reverse process, anhydrous form A transforms to the tetrahydrate directly. On the other hand, an intermediate state appears in the adsorption process of anhydrous form B as is the case of guanosine [2]. By comparison of the crystal structure of the tetrahydrate with those of anhydrous forms A and B, it is concluded that interfacial and strain energy contributions in the nucleation process at the transition point are dominant factors in bifurcation, hysteresis, and emergece of the metastable states observed in the phase transitions.

[1] Sugawara Y., et al., *J. Phys. Chem.* B, 2002, **106**, 10363. [2] Urabe H., Sugawara Y., Kasuya T., *Phys. Rev.* B, 1995, **51**, 5666.

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