Phase Behavior of Water inside Protein Crystals

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Protein crystals typically consist of 40 - 60 % water. The internal water forms solvent channels (2 - 4 nm in diameter) inside the crystals. We have studied the phase behavior of water inside protein crystals using a novel crystal freezing method: high-pressure cryocooling. Using X-ray diffraction, we demonstrated that the high-density amorphous (HDA) ice induced inside the high-pressure cryocooled protein crystal undergoes a phase transition to low-density amorphous (LDA) ice as the crystal is warmed from 80 to 170 K. We found that the intermediate states in the temperature range from 80 to 170 K can be reconstructed as a linear combination of HDA and LDA ice, suggesting a first-order transition. We also found evidence for a liquid state of water during the ice transition by monitoring the protein crystallographic data, suggesting a glass transition of HDA ice. These results provide new insights into the anomalous behavior of supercooled water and open a host of unanswered questions.

References

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