

Order and Disorder in Lysozyme Crystals Caused by the Phase Transition

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Some lysozyme crystals transform to low-solvent crystals by dehydration-induced phase transition [1], [2]. The transition took several hours and the change of X-ray diffraction was recorded to monitor the process [2]. Strong diffuse streaks were observed in the intermediate state where the crystal contains two types of micro-crystals, one with the native lattice and the other with the transformed lattice. At the end of the transition, the transformed micro-crystals were re-ordered as indicated by disappearance of the diffuse streaks. However, the relatively large mosaicity and distinct diffuse scattering indicated that the order of the micro-crystal as well as the crystal packing was not fully recovered.

The structures of native and transformed crystals were determined at resolution 1.13-1.16 Å. They shared essentially the same backbone structure between native and transformed crystals. In the triclinic crystal, however, a conformational change in the main chain was observed in the large loop region of Ser60-Leu75, where a sodium ion was bound in the transformed crystal in place of water molecules in the native crystal. The peptide plane linking Arg73 and Asn74 was rotated 180° in the transformed crystal. In contrast, a sodium ion bound in the monoclinic crystal was removed in the transformed crystal where the corresponding loop region showed a water-bound structure.

[1] Kodandapani M.R., Vijayan M., *Acta Cryst.*, 1993, D49, 234. [2] Harata K., Akiba T., *Acta Cryst.*, 2004, D60, 630.

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