Poster Presentation

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Temperature-dependent structural change of 1D ice, water nanopipe, in crystal

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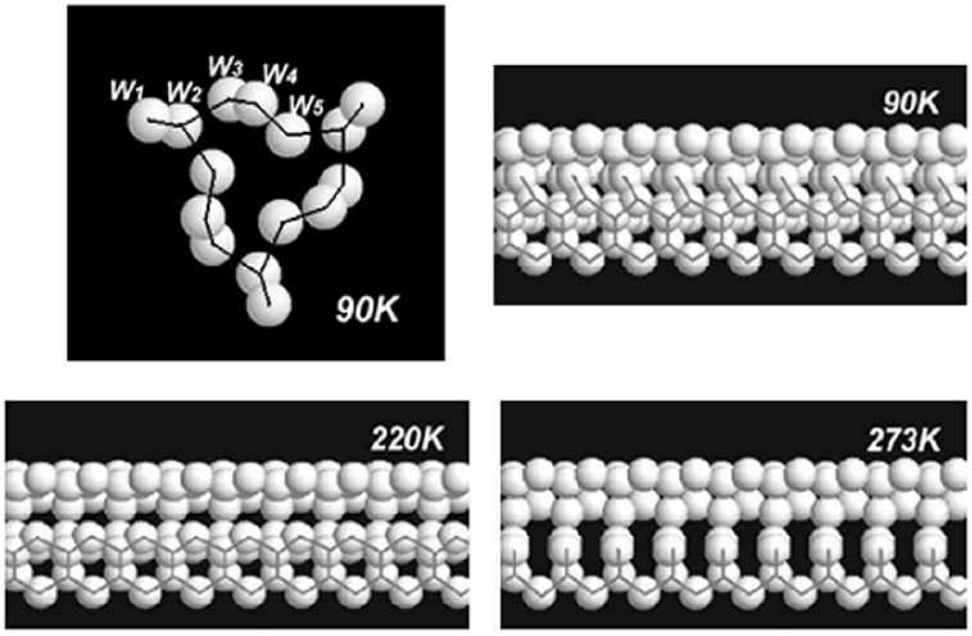
One-dimensional ice (1D ice) is formed in the single crystal prepared by mixing tryptophan and pyridoxal-5-phosphate in aqueous solution. This ice (diameter=1.649nm at 90K) consists of a hollow-type nanowire, viz., water nanopipe, and the structure is constructed by piling up the cluster unit of 15 water molecules, five independent waters (W1,--W5) of which are arranged around a 3-fold axis. As can be seen from the side view of this nanopipe, a tape structure is made of the continuous chair-type six-membered rings running parallel to the longest crystal axis, and its three tapes arranged around 3-fold axis are linked together via two kinds of hydrogen bonds of W5 (W5-W2 and W5-W4). Thus, the overall structure of this 1D ice could be described as three-square nanometric column. In order to investigate the temperature-dependent structural change of 1D ice, the crystal structure was refined using the X-ray diffraction data measured at different temperature between 90K and 293K. From these results, it was confirmed that the nanopipe structure is stable under 200K, but W5 and W4 disappear at 220K and 273K, respectively, indicating the importance of W5 for the structural stability of 1D ice.



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