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Observation of phase change from H2O ice VI to ice VII using molecular dynamics calculation

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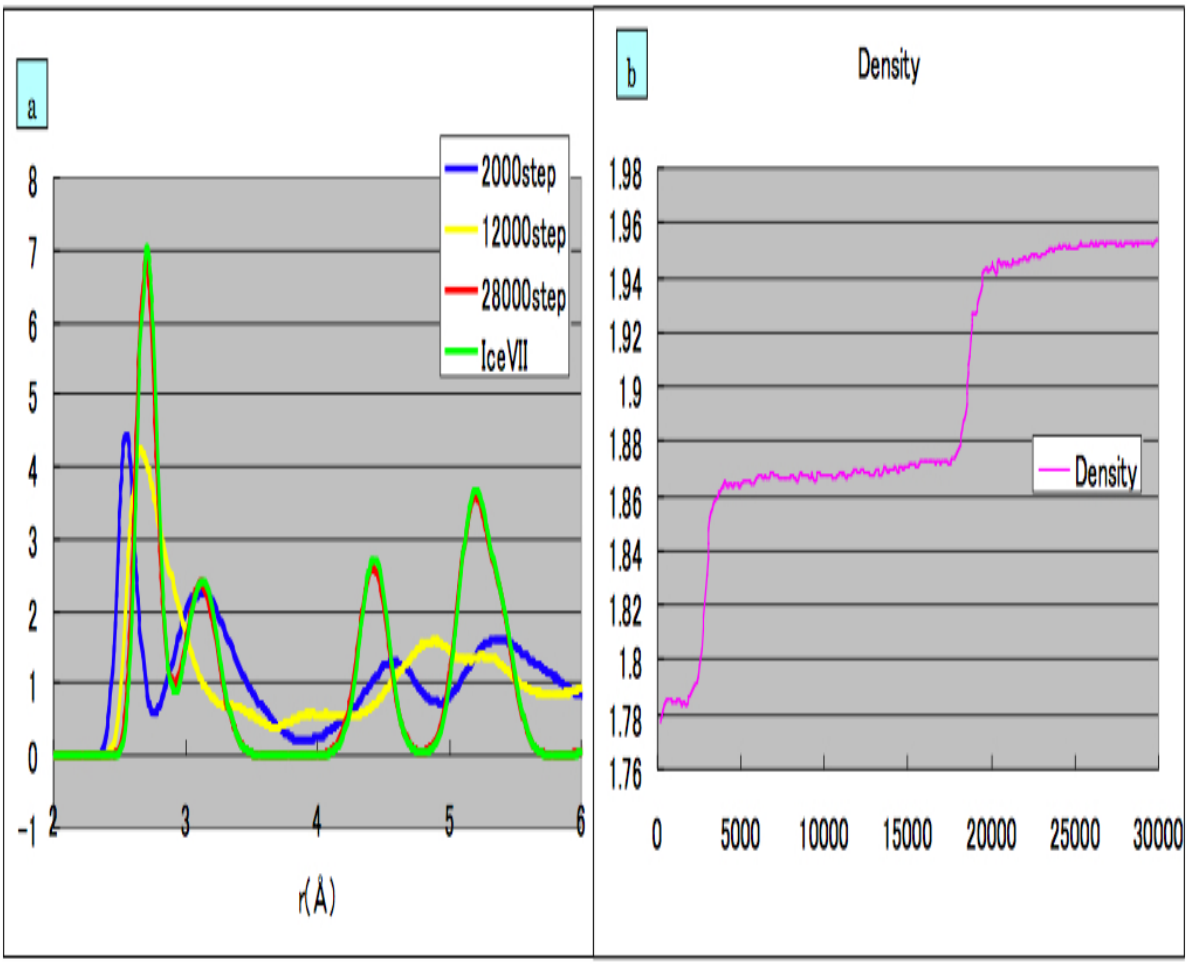
Figure (a) Distribution function of oxygen – oxygen of ice VI (2000 steps), an unknown intermediate structure (12000 steps) and ice VII (28000 steps and reference ice VII). (b) Density change from ice VI through an intermediate structure to ice VII. This calculation is a result at 20 GPa and 300 K.



We find a phase change from H_2O ice VI to ice VII through an unknown intermediate structure at 20 GPa and 300 K (Figure) using MXDORTO program developed by Dr. K. Kawamura at Tokyo Institute of Technology (Hirao and Kawamura, 1994, Material Design using Personal Computer, Shokabo publishing, P. 230) and potential parameters of H_2O suggested by Dr. K. Kawamura (Teion Kagaku 2005). In real world, ice VI changes its structure to ice VII at 2 GPa and 300 K. This calculation demonstrates prediction ability of MD calculation and importance of potential parameter to fit quantitative values.

Keywords: water, ice, high pressure, molecular dynamics, molecular simulation, H2O