

Improvement of web-based educational tool to understand the state change of water in atomic scale

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<http://akebono.ei.kochi-u.ac.jp/~akamatsu/>

A Web-based educational tool to understand the state change of water in atomic scale was developed and improved. This tool reproduces the melting of ice and the vaporization of liquid water, showing the 3D-animation of H₂O molecules as the result of molecular dynamics simulation. In the animation of melting, the hexagonal arrangement of water molecules is observed to collapse. In the vaporization, the increase of volume (= density decrease) is clearly shown.

You can easily reach to the high spot of melting or vaporization through Internet:

<http://akebono.ei.kochi-u.ac.jp/~akamatsu/H2O/> (Kochi University)

<http://chigaku.ed.gifu-u.ac.jp/chigakuhp/html/kyo/1/H2O/> (Gifu University)

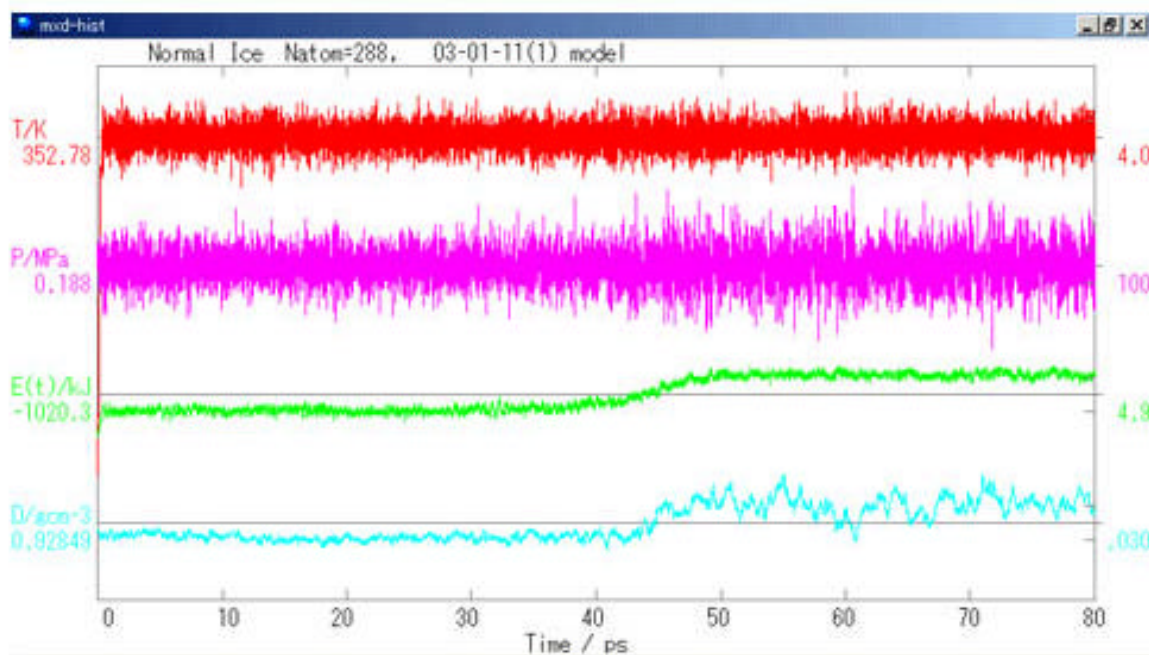
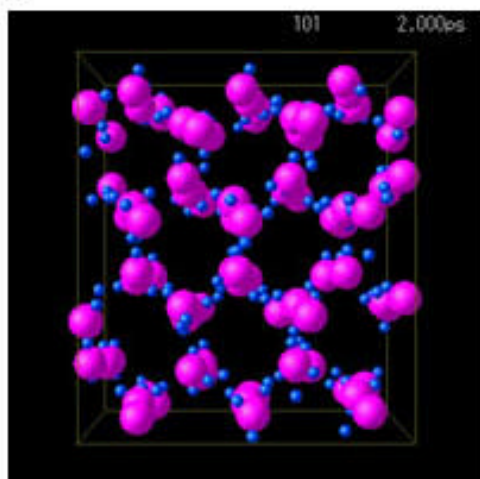


図1. 氷の融解計算における温度 T , 圧力 P , 内部エネルギー E , 密度 D の履歴. 96 個の H_2O 分子 (=192 個の H 原子 + 96 個の O 原子) からなる氷を, 80°C (= 353 K) に保持したところ, 約 40 ps (= 40×10^{-12} 秒) 後に融解が始まり, 内部エネルギーおよび密度の上昇が起きた.

(a)



(b)

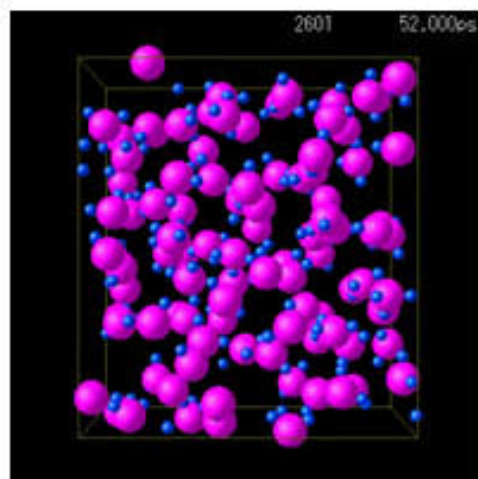


図2. 氷および水についての静止画像. (a) 融解する前の氷. (b) 融解直後の水. Web ページ上のアニメーションにおいては, 氷や水を作っている H 原子 (小さな玉) と O 原子 (大きな玉) とが激しく動いている様子を眺めることができる.