A Molecular Dynamics Simulation of Adsorption of Molecules in Nanotubes

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Since the epoch-making expectation of hydrogen storage capacity with SWNTs by Dillon et al. [1], the physical mechanism of hydrogen storage with carbon materials has been intensively studied. In our previous molecular dynamics studies of the hydrogen physical adsorption with a small bundle of SWNTs, it was concluded that the hydrogen storage capacity could not by high enough as the commercial automobile application unless the system temperature was cooled down to 77 K [2].

In this report, the effect of various geometrical structures of carbon materials on the physical adsorption of hydrogen and other gas molecules was studied with the classical molecular dynamics simulations. As an example, the potential field for hydrogen in the tip of carbon nanohorn [3] is shown in Fig. 1. Some strong adsorption area at the tip was expected. The effect of effusion with carbon nanohorn is also discussed. As other geometrical possibilities, MWNTs and strained SWNT will be examined. Furthermore, in order to estimate the physical adsorption characteristics of other molecules with such carbon structures, arbitrary different interaction potential between carbon and molecules are studied.

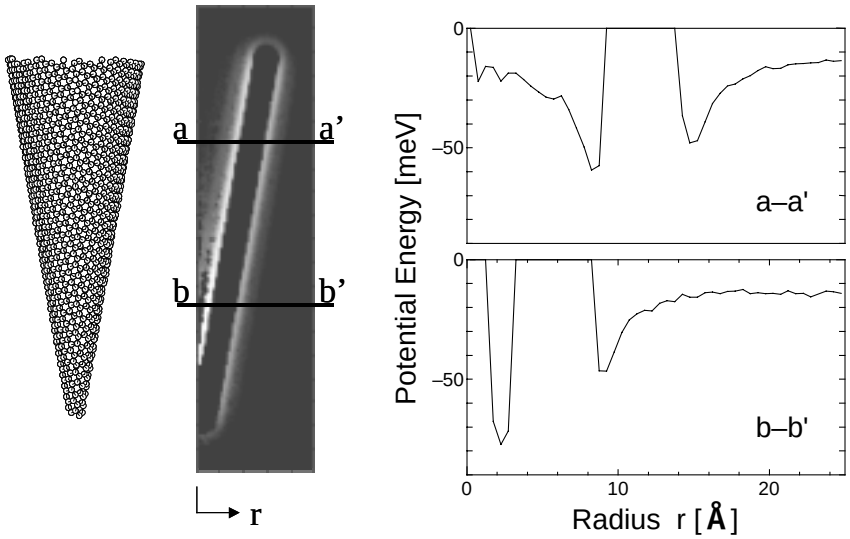

Fig.1 Potential energy distribution of hydrogen in the tip of a carbon nanohorn for 77K and 12MPa.

References

[1] A. C. Dillon et al., *Nature*, 386-27, 377, (1997).
[2] S. Maruyama and T. Kimura, *Proc. ASME HTD*, 2, 405 (2000).
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