The Search for Advanced Functional Materials concern with “Eco-products”

Project Representative

Takashi Yoshida

Corporate Research and Development Center, TOSHIBA Corporation

Authors

Takashi Yoshida[*1], Misako Iwasawa[*2]

＊1　Corporate Research and Development Center, TOSHIBA Corporation

＊2　Japan Agency for Marine-Earth Science and Technology

Abstract

It produces nano-scale fabrication by using wet-process procedures. It is plausible grasp that solvent molecules and etching residues (clusters or molecules) are contained in confined nano-spaces. In these situations, it is possible unique discrepancies observing between a macro scale dynamics that solute molecules (or particles) dynamics in confined solution systems. For the solvent and solute dynamics are analyzed for nanometer scale systems, molecular dynamics (MD) simulations are very useful calculation methods. And, it is possible that the free energy differences for the diffusion of solutes derived from MD simulations.

In this work, we applied self-consistent histogram method [1] for the calculations of free energy differences using MD simulations, as follows equations.

$$P_0^{est}(Q) = \frac{\sum_{i=1}^{n} H_i(Q)}{\sum_{i=1}^{n} \exp(-\beta W_i) M_i Z_0 / Z_i}$$

$$Z_i = \int dQ \exp(-\beta W_i) \frac{\sum_{j=1}^{n} H_j(Q)}{\sum_{k=1}^{n} \exp(-\beta W_k) M_k / Z_k}$$

For our free energy calculations of two model systems, which are a LJ-particle in solid/liquid/vacuum system and an ion pair into the filling water solvent in nano-channel system, were applied above equations, that self-consistent formula rewrites to the recursive formula by applying some expectations. All calculations of this study were carried out using the MD program package of LAMMPS [2].

Keywords:　nano-fabrications, molecular dynamics simulations, interface, free energy calculation

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