

Simulation of chemical reaction by the generalized ensemble method

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We developed a new simulation method for calculating the properties of chemically reactive systems. In the chemical reaction on a certain size molecules, especially polymers, the most important role is played by the elementary reaction, but also other factors influence the behavior of the whole process, which are a contact frequency between reactive sites, steric effects of molecules, and diffusion of molecules. In order to estimate these effects, we use a combination of molecular dynamic method and Monte Carlo method under the conventional molecular force field. In the rearrangement of bonds in the elementary reaction, the molecular force field is different in reactant and product. Therefore Metropolis decision may be evaluated incorrectly. To overcome this problem, we improve the Wang-Landau method, which is a kind of generalized ensemble method, to simulate between different Hamiltonians. Our method is based on the equilibrium distribution. Then the target is equilibrium reactive system or slow reactive system, such as the polymerized system of polymer.