Large-scale Simulation for Catalyst Chemical Vapor Deposition

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Abstract

Rare metal has been consumed by the advanced technologies and the products which support our country.

In order to prepare for the risk for the resources, we should develop alternative materials for the rare metal. This project is aimed to develop a new catalyst for the alternative of the rare metal by a computational approach with a help of experimental analysis.

This year, we focus on the behavior of the Fe catalyst in the chemical vapor reaction which is related to the synthesis of the single wall carbon nanotube. Utilizing multi-scale modeling by combining a large-scale classical molecular dynamics and a first principle calculation, we examined the detailed mechanism and the main control factors of the growth of the carbon nanotube through the pursuit of the complex catalyst reaction process.

A classical molecular dynamics code named DL_POLY and a first principle molecular dynamics code named PWscf were used for the analysis of the generation and the growth process of the carbon nanotube, and for the analysis of the decomposition of the hydrocarbon on the Fe catalyst, respectively. For the DL_POLY code, a new function which changes the inter-atomic potential depending on the particle arrangement was introduced. In addition, the code was optimized for the vector operation of the earth simulator that enables a very large scale calculation.

As a result, we confirmed the decomposition process of the methane on the surface of the iron catalyst and the diffusion of the decomposed carbon in the iron catalyst in good agreement with the VLS reaction process model we advocate.

Keywords: catalyst reaction, classical molecular dynamics, first principle molecular dynamics, VLS reaction process model