Study of the Automatic Modeling of Reaction Systems for Chemical Vapor Deposition Processes using Genetic Algorithms

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To identify reaction models is very helpful for developing Chemical Vapor Deposition (CVD) processes. However, the automation of the works for identifying the reaction models is obstructed, because there are many intellectual procedures in them. Therefore, we proposed the novel technique, as we called Evolutionary Analysis for Reaction Systems (EARS), for determining appropriate reaction models by analyzing experimental data automatically using Genetic Algorithms (GA) (1).

Figure 1 (a) shows the conventional modeling method of reaction systems (2). Appropriate reaction models are drawn from experimental data by solving the reverse problems of reaction processes. Figure 1 (b) shows the modeling method that we proposed on the basis of the theory of evolution. In the first place, the candidates of the appropriate reaction model were set at random or *a priori*. Then, the predicted (simulated) results corresponding to the experiment results were calculated from the candidates of the reaction models by solving forward problems of the reaction processes. Next, the amount of the difference between the predicted results and the experimental results was estimated. The more different is the candidate of the reaction model from the appropriate reaction model, the larger is the amount of the difference between the predicted and the experimental results. At last, the candidates of the reaction models were modified on the basis of the theory of evolution, that is, by evolutionary computing using the amount of the difference as the evolutionary pressure. These procedures were repeated until the amount of the difference became small enough. We adopted the GA as the method of the evolutionary computing, because the GA is robust and suitable for global optimizations.

Figure 2 shows the example of the reaction models. The appropriate reaction models were determined both quantitatively and qualitatively, based on chemical kinetics. The reaction models consist of deposition species (including source gases), films, gas-phase reactions with the values of the rate constants kg, and surface reactions with the values of the rate constants ks. Arrows indicate the gas-phase reactions and the surface reactions, and the directions of arrows correspond to the directions of the reactions. Both the gas-phase reactions and the surface reactions imply the first-order reactions of the deposition species. The reaction models were expressed by the combinations of the states of them, that is, on and off for the deposition species, and the surface reactions, forward, backward, and off for the gas-phase reactions. All patterns of the combinations were considered, although the maximum number of the deposition species was restricted to four, and the values of the rate constants were limited to the range that we defined.

Figure 3 shows the schema of the automatic modeling system. The system consists of three devices, that is, a user interface, an inference engine, and virtual reactors (reaction simulators). The inference engine proposes the reaction models, examines the validities of them, estimating the difference between the predicted and the experimental results, by operating the virtual reactors for itself, and corrects the models using GA. In order to take the appropriate reaction models, only users have to do is to input the information of the experimental data with the experimental conditions to the system through the user interface.

We investigated the ability of the system by use of the experimental data of tetraethylorthosilicate (TEOS) thermal CVD (2). We successfully showed that the system enough ability to identify the reaction models appropriately from the experimental results of CVD. Therefore, the conventional procedures of reaction modeling can be replaced with the system, and the system will contribute to the automation of R&D works.

Reference

1. J. H. Holland, Adaptation in natural and artificial systems, University of Michigan Press (1975).
2. T. Sorita *et al., J. Electrochem. Soc.* **140** 2952 (1993).

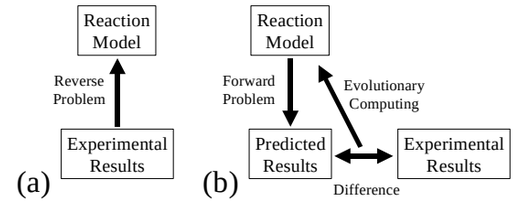

Figure 1. Comparison of the modeling methods (a) Conventional method (b) Evolutionary method

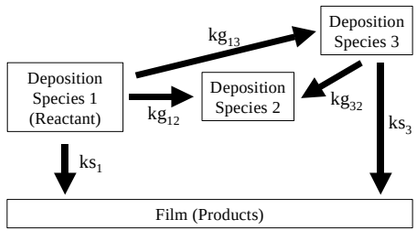

Figure 2. Example of reaction model

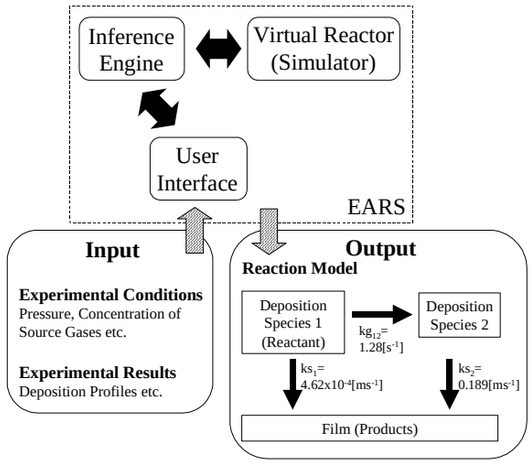

Figure 3. The schema of automatic modeling system