Development of the automatic modeling system for reaction mechanisms using REX+JGG

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Abstract

The identification of appropriate reaction models is very helpful for developing chemical vapor deposition (CVD) processes. In this study, we developed an automatic modeling system that analyzes experimental data on the cross-sectional shapes of films deposited on substrates with nanometer- or micrometer-sized trenches. The system then identifies a suitable reaction model to describe the film deposition. The inference engine used by the system to model the reaction mechanism was designed using real-coded genetic algorithms (RCGAs): a generation alternation model named “just generation gap” (JGG) and a real-coded crossover named “real-coded ensemble crossover” (REX). We studied the effect of REX+JGG on the system’s performance, and found that the system with REX+JGG was the most accurate and reliable at model identification among the algorithms that we studied.

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Selection and peer-review under responsibility of Organizing Committee of EUROCV 19.

Keywords: Chemical Vapor Deposition; Reaction Mechanism; Genetic Algorithms; Real-Coded Genetic Algorithms; Automatic Modeling; Simulation.

1. Introduction

CVD is one of the most important manufacturing processes used in the semiconductor industry. An important development in CVD processes is the identification of an appropriate reaction model (reaction mechanism) to indicate the reaction paths from the reactants (source gases) to the products (films), both

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quantitatively and qualitatively [1]. In addition, considerable information about the reaction model can be obtained from experimental results on the deposited film shapes, such as the cross-sectional shapes of films formed on substrates with nanometer- or micrometer-sized trenches [2,3]. Therefore, to accelerate the development of CVD processes and decrease the labor required for determining reaction models, we developed an automatic modeling system that can determine the reaction mechanisms involved in CVD processes by analyzing the shapes of films deposited on substrates with trenches [4,5]. The system was designed through the use of both simple and real-coded GAs [6,7], because these are robust and suitable for global optimization. We demonstrated that our system could successfully identify the correct reaction models corresponding to synthetic experimental results. However, the system is at an early stage of development and more powerful modeling algorithms are needed to deal with complex reaction systems and a wider range of experimental data. The modeling algorithm REX+JGG, which combines the generation alternation model JGG with the real-coded crossover REX, is one of the finest and most powerful algorithms among the RCGAs for real parameter-optimization problems [8]. We believe that the performance of our reaction modeling system will be improved by implementing REX+JGG. Therefore, in this study, we developed an automatic modeling system that incorporates REX+JGG and investigated the effect of these algorithms on the quality of the modeling results for the reaction mechanisms.

2. Computational details

2.1. Process simulator and experimental results

We adopted a film deposition simulator based on the simple Monte Carlo (SMC) method [1,9,10] as a component of the modeling system, to obtain the infinite shapes of cross sections of the films formed on substrates with nanometer- or micrometer-sized trenches. We designed the simulator calculation process using partial least squares (PLS) regression analysis [11], to decrease the simulator calculation time [12,13]. Figures 1 and 2 show examples of the simulated shapes of the films deposited in the trenches, along with definitions of the various indices used in the figures to represent the characteristics of the trench and the deposited film. The cross-sectional shape of the trenches was assumed to be trapezoidal. With regard to the experimental results, we used the step-coverage and coverage ratios for film uniformity and the filling ratio of a trench for the filling property. We described details of the simulator and experimental results in our previous papers [4,5].

![Fig. 1. Cross-section of film deposited in trench, and indices for film uniformity.](image)

\[
\begin{align*}
A_t &\equiv T_h / T_b \\
S_t &\equiv F_b / F_t \\
C_x &\equiv F_x / F_t \\
R_t &\equiv F_t / (\min(T_t, T_b))
\end{align*}
\]
2.2. Reaction model

Appropriate reaction models were determined both quantitatively and qualitatively on the basis of chemical kinetics. The reaction models consisted of deposition species (including source gases), films, and surface reactions with a sticking coefficient value. In the models, the gas-phase reactions of the deposition species were assumed to be negligible because the films were deposited under the conditions of a Knudsen diffusion regime. The surface reactions in the models were first-order reactions of the deposition species. The maximum number of deposition species was restricted to four, and the values of the sticking coefficients were limited to the range that we defined. The model is thus a subset of the complete reaction model including gas-phase reactions [14]. Because the calculation cost for our model is much lower than that for the complete model, our model is suitable for investigations of the performance of the RCGAs implemented in the system.

2.3. Automatic modeling system

Figure 3 shows the schema of the automatic modeling system that we developed previously [4,5]. The system consists of three components - a user interface, an inference engine, and a virtual reactor (i.e., process simulator) - that reproduces film shapes. The inference engine proposes a reaction model, examines its validity by comparing the experimental results with the predicted ones obtained using the virtual reactor, and then corrects it using RCGAs. Therefore, the quality of the model proposed by the system depends heavily on the performance of the RCGAs.
2.4. RCGAs and modeling method

We compared two calculation methods for RCGAs; the specifications of these methods are shown in Table 1. BLX-alpha is a conventional RCGA method using blend crossover, which is a two-parental crossover operator [7]. We used BLX-alpha as a reference. REX+JGG is a novel type of RCGA that uses an advanced generation alternation model [8]. The multiparental crossover operator is more suitable for the optimization of multidimensional vectors, such as the information on the reaction models, than is the two-parental operator. REX is one of the multiparental crossover operators, in which the statistics of the parents are preserved. REX generates the children (candidate vectors for the reaction model) from the information on the parents as follows.

\[
z^c = z^g + \sum_{j=1}^{n+k} \xi_j (z_j - z^g)
\]

(1)

JGG is one of the generation alternation models, and it is optimized to the multiparental crossover operators. Parent chromosomes extracted by JGG are completely replaced with child chromosomes produced by the crossover operators.
Table 1. Specifications of RCGAs.

| Method       | Operators for RCGAs                                                                 |
|--------------|-------------------------------------------------------------------------------------|
| BLX-alpha    | Blend crossover, Uniform mutation, Tournament selection with elite strategy         |
| (See Ref. 7) |                                                                                     |
| REX+JGG      | REX (Real-coded ensemble crossover), JGG (Just generation gap)                       |
| (See Ref. 8) |                                                                                     |

We applied the value $r$ of the fitness function to the RCGA calculations to estimate the differences between the predicted and experimental results as follows.

$$r = \sqrt{\frac{\sum (v_{exp_i} - v_{calc_i})^2}{\sum v_{exp_i}^2}}$$  \hspace{1cm} (2)

Figure 4 shows an outline of the modeling method based on the theory of evolution [4]. First, the candidates for the appropriate reaction model were set at random or a priori. The predicted (simulated) results corresponding to the experimental results were then calculated from the reaction model candidates by solving the forward problems of the deposition processes using the SMC method. Next, the difference between the predicted results and the experimental results was estimated using equation (2). Based on our work, we believe that the greater the difference between the predicted and the experimental results, the greater the divergence between the candidate reaction model and the optimum reaction model. The reaction model candidates were then modified on the basis of the theory of evolution; that is, by RCGAs using the magnitude of the difference, which is described by the fitness value function in equation (2) as the evolutionary pressure. These procedures were repeated until the difference between the predicted and actual results became smaller than the limit that the users set beforehand. In addition, we added a function that indicates the simplicity of the models to the fitness value function, because simple reaction models are generally preferable to more complicated ones [4,5].

Fig. 4. Outline of modeling method.
3. Results and discussion

To investigate the validity of our automatic modeling system, we used a synthetic experimental data set that included the values of the step-coverage, coverage ratios, and filling ratio created from the original models represented in Figure 5, along with various flux ratios of the deposition species and various specifications of the trenches, as shown in Table 2. The modeling system is considered to have successfully modeled a reaction mechanism if the system analyzes the synthetic data and proposes the same reaction model as the original one. Therefore, we inputted the synthetic experimental data set into the modeling system and searched for appropriate reaction models in a qualitative as well as a near-quantitative manner.

**Fig. 5. Synthetic reaction model.**

![Synthetic reaction model](image)

**Table 2. Specifications of trench.**

| Trench No. | Aspect ratio $A_s$ | Tilt of side wall $\theta$ | Thickness ratio $R_t$ |
|------------|-------------------|-----------------------------|----------------------|
| 1          | 1.895             | 8.409                       | 0.23688              |
| 2          | 2.217             | 8.872                       | 0.27713              |
| 3          | 3.485             | 22.614                      | 0.48792              |
| 4          | 2.154             | 27.631                      | 0.40689              |
| 5          | 2.304             | 11.499                      | 0.28800              |

The system was able to successfully determine the correct reaction models within 50 generations for both BLX-alpha and REX+JGG calculations. Figure 6 shows a comparison of the reaction models proposed by the two RCGAs with the original (the answer). Although both of the proposed models were qualitatively and near-quantitatively in good agreement with the original one, the calculations by REX+JGG outperformed those of BLX-alpha with respect to the accuracy of model identification. To check the reproducibility of the proposed models, we compared the experimental results calculated from the proposed models with those from the original one. The mean errors between the original and the proposed models were as small as 0.498% and 0.061%, for BLX-alpha and REX+JGG respectively, and the maximum errors were 2.455% and 0.338%, for BLX-alpha and REX+JGG respectively. Therefore, the system using REX+JGG showed a better performance than the one using BLX-alpha.
Figure 7 shows the relation between the best fitness values and the generation of topological chromosomes for the RCGA calculations [14]. The fitness values for both BLX-alpha and REX+JGG gradually decreased—that is, became better—when the number of generations increased. However, the fitness value of BLX-alpha prematurely converged to a relatively higher position.

Overall, we can conclude that the system using REX+JGG outperformed the one using BLX-alpha with respect to both the accuracy and the convergence stability of the calculations.
4. Conclusions

We have developed an automatic modeling system, tested using BLX-alpha and REX+JGG, for determining the reaction mechanisms involved in CVD processes. The system works by analyzing the experimental results for the shapes of films deposited on substrates containing trenches. Although the system successfully identified the correct reaction models corresponding to synthetic experimental results, REX+JGG showed a greater potential for accurately and reliably finding the appropriate reaction models than did BLX-alpha.

Nomenclature

| Symbol | Description |
|--------|-------------|
| $A_x$  | aspect ratio of trench [-] |
| $C_x$  | coverage ratio at $x$ [-] |
| $E$    | filling ratio in trench [-] |
| $F_b$  | film thickness at bottom of trench [m] |
| $F_t$  | film thickness at top of trench [m] |
| $F_x$  | film thickness at $x$ [m] |
| $i$    | index of deposition species [-] |
| $j$    | index of parent for REX [-] |
| $k$    | incremental number of parents for REX, which are used with $n$ parents [-] |
| $n$    | dimension of chromosome; that is, of information on the reaction model [-] |
| $r$    | fitness value to GA calculations [-] |
| $R_t$  | ratio of film thickness to size of trench [-] |
| $S_t$  | step-coverage [-] |
| $T_b$  | width of trench at bottom [m] |
| $T_h$  | height of trench [m] |
| $T_t$  | width of trench at top of trench [m] |
| $U_i$  | flux ratio of the $i$-th deposition species [-] |
| $v_{exp,x}$ | index for experimental result, such as step-coverage and coverage ratio at $x$ [-] |
| $v_{calc,x}$ | index for calculated result corresponding to $v_{exp,x}$ [-] |
| $x$    | index of measured point in trench [m] |
| $z$    | $n$-dimensional vector for reaction model used as a parent of REX [-] |
| $z'$   | $n$-dimensional vector for reaction model generated by REX [-] |
| $z^e$  | center of gravity of parents for REX [-] |
| $\eta_i$ | sticking coefficient of $i$-th deposition species [-] |
| $\theta$ | tilt of side wall of trench [degrees] |
| $\xi$  | variable generated from probability distribution, where variance is $1/(n+k)$ and expected value is zero [-] |

Acknowledgements

This work was supported by KAKENHI (23560919).

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