Prediction Modeling for Ingot Manufacturing Process Utilizing Data Mining Roadmap Including Dynamic Polynomial Neural Network and Bootstrap Method

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Abstract. The purpose of this study was to develop a process management system to manage ingot fabrication and the quality of the ingot. The ingot is the first manufactured material of wafers. Trace parameters were collected on-line but measurement parameters were measured by sampling inspection. The quality parameters were applied to evaluate the quality. Therefore, preprocessing was necessary to extract useful information from the quality data. First, statistical methods were used for data generation, and then modeling was performed, using the generated data, to improve the performance of the models. The function of the models is to predict the quality corresponding to control parameters.

1 Introduction

Wafer is an important material in semiconductor industries. In recent years, the size of wafers has been enlarged up to 300 mm, so quality management is fundamentally required and applied. The wafer manufacturing process includes some chemical processes, so there is a time delay that causes difficult measurement and control. Among these processes, ingot fabrication is the most important, because the quality of the ingot will definitely affect the quality of the wafer.

Over decades, many studies have been performed to detect faults and improve yield. An adaptive resonance theory network was used to develop an intelligent system that will recognize defect spatial patterns to aid in the diagnosis of failure causes [1]. A data warehouse approach to the automation of process zone-by-zone defect-limited yield analysis [2], and SOI wafer-specific behavior related to the intrinsic limitations of laser-scattering defect detection were presented [3]. The calculations and results of random defect-limited yield (DLY) using the deterministic yield model was introduced [4], and the spatial defect features and cluster chip locations having similar defect features were extracted through the SOM neural network [5]. An auto-

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matic, wafer-scale, defect cluster identifier [6] and Geodesic Active Contours on a wafer-scale image were studied to extract the overall dimensions of the wafer under inspection [7].

The objectives of these studies were focused on detecting faults and adjusting the operational conditions for process optimization and producing wafers having no defects. To detect a fault, data mining tools to analyze input-output data using models are required. However, it is difficult to select a proper method from various data mining methodologies. In this research, a data mining roadmap was made to assist the selection of an appropriate methodology. Based on the roadmap, the selected methodologies were the data model to predict process quality. After selecting the method, data acquisition from the target process is used in data mining, and the collected data should be sufficient in number and clean enough to perform the data mining. The data on the quality of the wafer, prepared for this research, were not sufficient because quality evaluation was performed according to a sampling inspection, not a total inspection. To solve these problems, the bootstrap method, an appropriate data preprocessing method, was used to generate data sufficient for a total inspection. Improvement in model performance was observed from the results.

In Section 2, we describe the target process, which is the ingot fabrication process, and in Section 3, we show one of the important results, the proposed road map for data mining. Section 4 explains the applied data mining techniques, and Section 5 shows the experimental results. Finally, Section 6 concludes the paper.

2 Wafer Fabrication

2.1 Wafer for Semiconductors

Wafers are used in manufacturing memory or non-memory semi-conductor chips. Several circuit masks are mounted on one wafer by UV rays or electron beams in assembly lines. As semiconductor technology has developed, the wafer size has been enlarged to mount more circuits on the wafer. Because semiconductor manufactures want to make larger-memory and non-memory chips, they require larger-diameter wafers and strict quality assessment from wafer manufacturers. To cope with these requirements, optimization of wafer fabrication is essential.

2.2 Ingot Data

Ingot is the first manufactured material in wafer fabrication. In ingot fabrication, some set-points for handling the position or rotation of ingots and control parameters are adjusted for quality management. These operating parameters play an import role in wafer quality and size control. Therefore, they should be properly handled for improvement of productivity and yield. The operating parameters were used as inputs in modeling in this study. The quality parameters consist of five concentration values, and six defect values. Four of these were used for outputs in modeling in this study.

3 Design of Data Mining Roadmap

3.1 Data Mining

Data mining techniques that are well suited to the purpose can improve process performance and product quality. Data mining, a procedure for extracting useful information from data, is composed of data selection, preprocessing, transformation, data mining and interpretation. When collected data is insufficient, a data selection and preprocessing procedure should be considered an important stage. The raw data used in this research were insufficient to train models because most of the data was obtained from sampling inspection. To overcome this problem, a statistical method such as the Monte Carlo/Bootstrap method was used to fill vacancies in the data.

3.2 Data Mining Roadmap

In this study, we proposed the roadmap for data mining. Figure 1 shows the proposed roadmap, which was constructed based on several reference books and papers. We selected the methods and procedures for diagnosis and optimization of the ingot process by referring to the roadmap. The selected methods of this study were data generation (bootstrap method) and prediction modeling (DPNN).

3.3 Application of Data Mining

3.3.1 Data Preprocessing in Reducing Data Effects

The collected data from assembly lines can be missed or limited to specific cases; thus, the quality data are not always uniformly distributed. Insufficient data results in unreliable prediction models in the modeling stage. To solve these problems, data preprocessing is required in order to add data and improve performance. In this study, the Bootstrap method, a type of Monte Carlo method, was applied to compensate leakage data caused by sampling inspection.

3.3.2 Data Modeling in Quality Prediction

In modeling prediction models, inputs of models can affect the performance of the models. Selection of inputs corresponding to data characteristics is necessary to improve model performance, because unnecessary inputs can have a strong influence on prediction results. Therefore, in this study, we selected the principal inputs that greatly influence model accuracy after modeling. For the function, we proposed the dynamic polynomial neural network (DPNN). The DPNN has the advantages that it requires only small computation, so it is very useful in modeling with high-dimension variables and a large amount of data. The other advantage is that this method can select essential inputs through the modeling stages.

3.4 Process Management System in Ingot Fabrication

The designed models and the extracted rules are integrated into the process management system. This system will play important quality management roles in ingot manufacturing. The quality will be predicted by models and the control parameters will be modified by rules on-line. In Fig. 2, the quality predictor is to predict quality of the wafer according to the control parameters and the parameter estimator decides how to adjust the control parameters to improve the quality corresponding to the predicted quality.

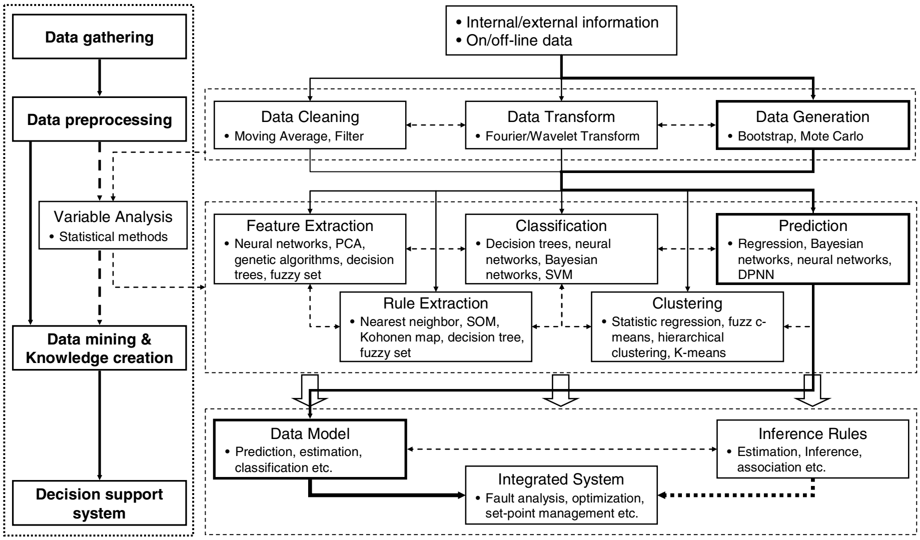

Fig. 1. Data mining roadmap proposed in this research

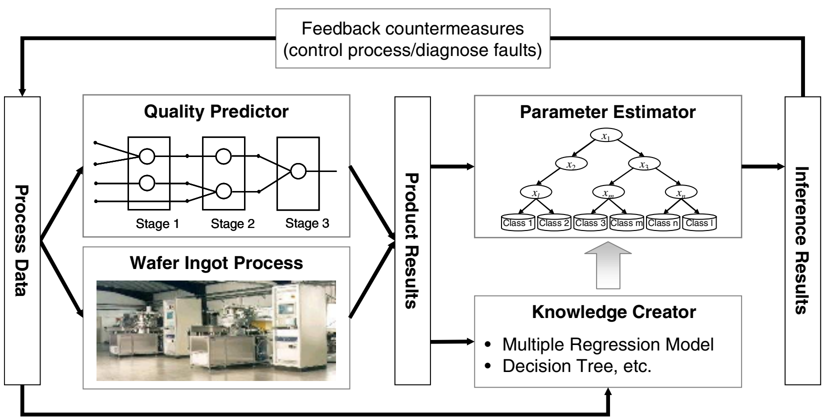

Fig. 2. Structure of the proposed system

4 Applied Data Mining Tools

The process data have limited characteristics. Trace data (control parameters) are collect by real-time measurement, but measurement data (quality parameters) are measured by sampling inspection after manufacturing. Therefore, input and output data cannot be one-to-one correspondent and target data are insufficient. The insufficient data problem results in modeling inadequate performance of the model because the target data are insufficient. To solve this problem, we used the Bootstrap method with data generation. After the data generation, the prediction model was constructed using the DPNN.

4.1 Bootstrap Method

The interested reader is referred to more information on the theory behind the bootstrap. Some studies refer to the re-sampling techniques of the previous section as bootstrap methods. Here, the term *bootstrap* is used to refer to Monte Carlo simulations that treat the original sample as a pseudo-population or as an estimate of the population. The bootstrap is a method of Monte Carlo simulation where no parametric assumptions are made about the underlying population that generated the random sample. Instead, the sample is used as an estimate of the population [8].

4.2 Dynamic Polynomial Neural Network (DPNN)

Polynomial neural network (PNN) based on the GMDH algorithm is a useful method to model the system from many observed data and input variables. It is widely employed for modeling of dynamic systems, prediction, and artificial intelligent control because of its advantages in data handling. Figure 3 includes the recurrent inputs with one-to-*n* time-delayed output variables [9-11].

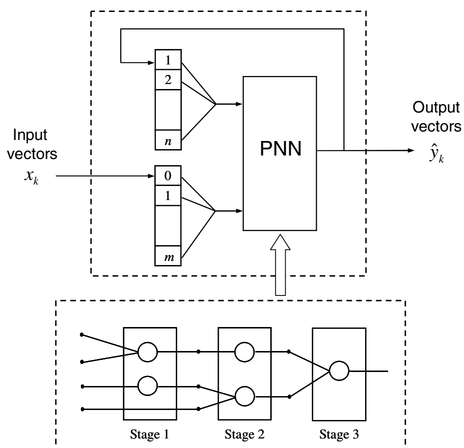

Fig. 3. Basic structure of DPNN

5 Experimental Results

5.1 Trace and Measurement Data of Ingots

Application data were collected from ingot fabrication on the company assembly line. Fourteen trace parameters and 11 measurement parameters that are used for quality analysis were included in the data sets. The trace parameter data are collected on-line.

The measure parameter data are gathered by sampling inspection and used for quality analysis. Forty-eight process parameters are collected by one data set per one minute from a puller.

The measurement parameter data were collected by sampling test, but the trace parameter data were gathered by on-line measurement. Thus, the insufficient data problem exists in modeling stage. The merging data from several pullers can be applied to solve the data insufficient data problem. However, each puller has a unique recipe, so the process features of each are different. Therefore, one puller data set was used with data addition based on data generation at the preprocessing stage. At the preprocessing stage, the number of the target data can be the same as that of the input data. Figure 4 shows the data interpolation.

Trace data (control conditions)											Measure data (product qualities)				
x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	x11	y1	y2	y3	y4	y5
18.00	1.20	0.11	56.20	5.00	204.91	75.55	24.40	18.03	17.97	114.88	15.04	-14.11	10.95	3.30	
17.98	1.04	0.12	56.20	5.00	204.84	77.15	24.40	18.00	17.94	114.90	11.57	-2.79	10.73	2.70	
18.00	1.08	0.12	56.30	5.00	205.25	78.15	24.60	17.97	17.91	114.91			10.71		
18.01	1.21	0.14	56.50	5.00	206.07	80.10	24.20	17.95	17.88	114.82	11.79	-5.85			
18.04	0.82	0.09	56.70	5.00	205.20	82.05	24.20	17.89	17.85	114.80			10.72		
18.03	1.38	0.11	56.70	5.00	206.01	83.45	24.60	17.87	17.82	114.76	•	•	10.69	•	
18.01	1.39	0.16	57.00	5.00	206.34	85.45	24.40	17.84	17.79	114.73	•	•	10.71	•	
18.01	1.45	0.17	57.10	5.00	206.86	87.40	24.20	17.81	17.74	114.70	•	•		•	
18.01	1.30	0.15	57.20	5.00	206.63	89.60	24.80	17.76	17.71	114.65			10.68		
18.01	0.96	0.15	57.50	5.00	206.63	91.55	24.60	17.73	17.68	114.64			10.67		
18.01	1.01	0.12	57.50	5.00	206.77	93.40	24.40	17.68	17.65	114.64			10.7		
18.00	0.98	0.11	57.60	5.00	206.50	94.50	24.60	17.65	17.62	114.61	•	•	10.68	•	
17.99	1.16	0.13	57.70	5.00	206.45	96.10	24.40	17.63	17.59	114.59	•	•		•	
18.00	0.84	0.14	57.90	5.00	206.50	97.95	24.60	17.60	17.56	114.54	•	•	10.69	•	
18.03	0.62	0.06	78.80	5.01	206.70	116.90	24.20	12.88	12.82	111.17			10.25		
18.01	0.62	0.06	78.80	5.03	206.79	116.85	24.20	12.85	12.79	113.12	11.47	-2.71	10.29	1.03	
18.05	0.62	0.06	78.90	5.02	206.83	116.90	24.20	12.82	12.79	113.09					
18.03	0.62	0.06	78.90	5.03	206.86	116.85	24.20	12.82	12.79	113.11			10.2		
18.04	0.62	0.06	79.10	5.04	206.87	116.85	24.20	12.82	12.76	111.30			10.19		

Insert Generated Data

Fig. 4. Data generation for unmeasured quality data

5.2 Quality Prediction and Variable Selection Using DPNN

The process of wafer manufacturing is a chemical process, so the product quality can be measured after fabrication. If the quality is predicted by current control conditions, the manufacturing process can be effectively operated. This section treats modeling stage selection that is based on the roadmap. In this study, we used a DPNN because the DPNN is a useful method for data modeling with many variables and data.

5.2.1 Data Modeling Using One Puller Data (Case 1)

Figures 5 to 6 show the test result using the trained DPNN model with unseen data. The prediction models were designed for quality prediction corresponding to Oxygen, ORG (Oxygen Gradient), RES (Resistivity), and RRG (Resistivity Gradient). In the RES case, the model can be designed by one puller data because the data are sufficient to design a model. And the model performance is also adequate to predict the quality of wafers with RES. However, other three-parameter data are not sufficient to design a good performance model. The model was not trained well with one puller data. Table 1 shows train and test results and selected inputs from modeling using one puller data.

5.2.2 Advanced Proposed Modeling Based on Data Generation (Case 2)

As mentioned above, insufficient data cannot construct a good performance model, so the preprocessing stage was required to compensate for weak points caused by insufficient data before applying the main data mining techniques. In this paper, we used the Bootstrap method to solve the data problem. The Bootstrap method is a type of Monte Carlo simulation. It can generate reasonable data to design data models and improve model performance. Figures 7 to 8 show the improved results that are achieved by data generation. Table 2 shows the prediction results and input selection. As shown in the results, AR gas flow, Chamber press and Heat power were selected.

5.2.3 Comparison of Performance of Prediction Models

Table 3 shows the comparison result for two modeling cases. In Case 1, the models were designed by one puller data that was insufficient in amount, so an overfitting problem occurred. This means that a model trained by insufficient data cannot ensure the good performance of models. However, in Case 2, the model trained stably by data addition using the Bootstrap method showed a good performance. The results provide on indication that statistical data generation can reduce the effect of the insuf-

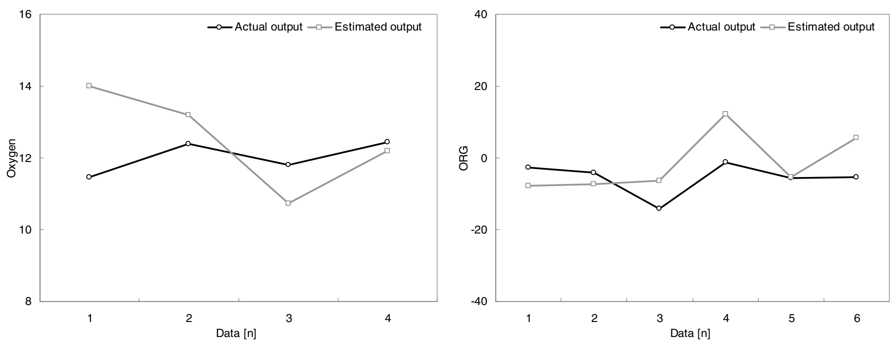

Fig. 5. Prediction result for Oxygen and ORG

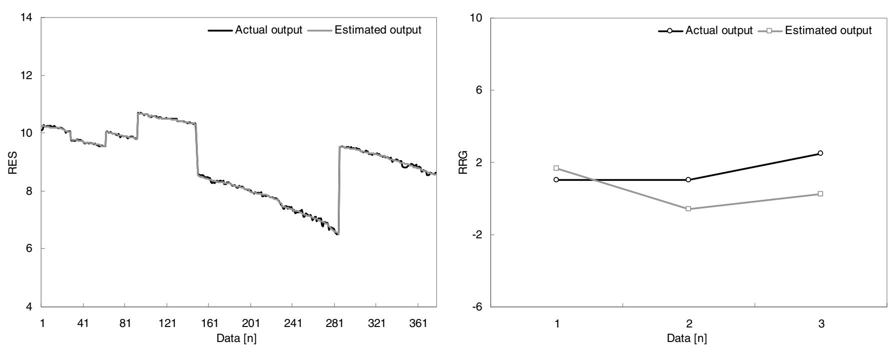

Fig. 6. Prediction result for RES and RRG

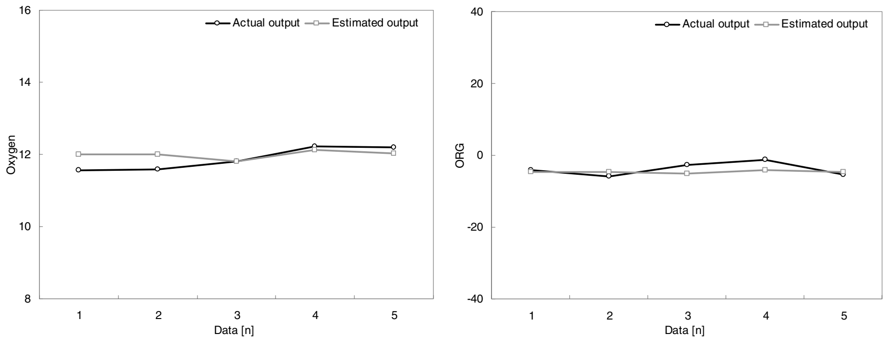

Fig. 7. Prediction result for Oxygen and ORG

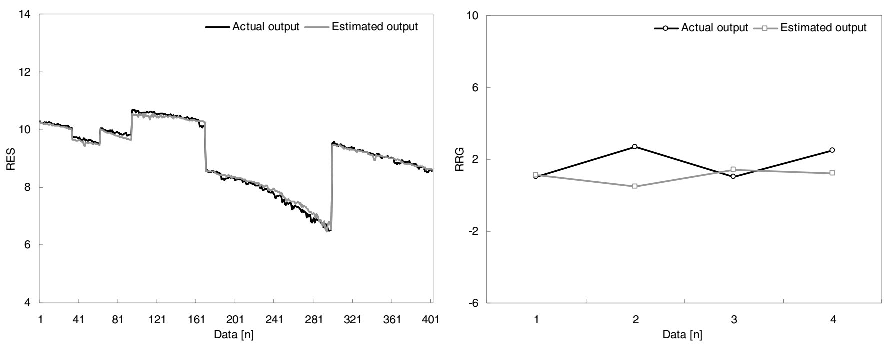

Fig. 8. Prediction result for RES and RRG

ficient data problem. It is difficult to analyze the relationship between inputs and outputs using field data because sometimes field data are insufficient for modeling. Therefore, data preprocessing is required. In this study, an adequately descriptive model was designed by data generation.

Table 1. Modeling results using one puller data including prediction and input selection

Value	Oxygen	ORG	RES	RRG
Learning error	9.7089e-015	4.8174e-014	0.0632	4.5275e-016
Prediction error	1.4422	8.0759	0.043938	1.6293
Selected layer	3	5	3	3
Selected inputs	1 4 5 9 10	2 3 4 5 6 9 10 11	3 4 6 7 9	2 3 4 5 10

Table 2. Modeling results with data generation including prediction and input selection

Value	Oxygen	ORG	RES	RRG
Learning error	0.4550	1.2730	0.3005	0.8512
Prediction error	0.29528	1.8733	0.10423	1.2942
Selected layer	4	4	4	3
Selected inputs	1 2 3 7 8 9 11	1 2 3 5 6 8 11	2 3 4 7 9 11	1 2 6 7 8 9 11

Table 3. Comparison results for three case data sets

Value	Case	Oxygen	ORG	RES	RRG
Learning error	1	9.7089e-015	4.8174e-014	0.0632	4.5275e-016
	2	0.4550	1.2730	0.3005	0.8512
Prediction error	1	1.4422	8.0759	0.043938	1.6293
	2	0.29528	1.8733	0.10423	1.2942
Selected layer	1	3	5	3	3
	2	4	4	4	3

6 Conclusions

In ingot fabrication, quality inspection is accomplished by product sampling testing, and then the control parameter is adjusted by an operator's action corresponding to the quality. Therefore, it is necessary to predict the quality with respect to current control parameters and to handle the parameters effectively.

However, it is difficult to design models using collected data from the field because the data are gathered by sampling inspection. In this study, we proposed data generation using the bootstrap method to solve insufficient data problem. And then we designed prediction models using the DPNN. Through the stages, the performance of the models could be improved and were reasonable. The final goal of this study was to integrate both the diagnosis and the optimization systems of the ingot fabrication process. By using the integrated management system, the quality can be predicted corresponding to the control parameters.

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