Estimation of Qualities and Inference of Operating Conditions for Optimization of Wafer Fabrication Using Artificial Intelligent Methods

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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. Operating data (trace parameters) were collected on-line but quality data (measurement parameters) were measured by sampling inspection. The quality parameters were applied to evaluate the quality. Thus, preprocessing was necessary to extract useful information from the quality data. First, statistical methods were employed for data generation, and then modeling was accomplished, using the generated data, to improve the performance of the models. The function of the models is to predict the quality corresponding to the control parameters. The dynamic polynomial neural network (DPNN) was used for data modeling that used the ingot fabrication data.

Keywords: Wafer fabrication, data mining, data model, process optimization

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 that management is essentially required and applied. The wafer manufacturing process includes certain chemical processes; there is a time delay that causes difficulty in measurement and control. Among the chemical processes, ingot fabrication is the most important, as the quality of the ingot will definitely affect the quality of the wafer.

Over decades, many studies have been performed for fault detection and yield improvement. An adaptive resonance theory network [1] was used to develop an intelligent system that will be able to recognize defect spatial patterns to aid in the diagnosis of failure causes. 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 [3], was presented. The modeling of wafer fabrication was carried out; the calculations and results of random defect-limited yield (DLY) using the deterministic yield model [4], the spatial defect features and cluster chip locations having similar defect features that were extracted through the SOM neural network [5], and an automatic, wafer-scale, defect cluster identifier [6] and Geodesic Active Contours on a wafer-scale image to extract the overall dimensions of the wafer under inspection [7]. An advanced methodology using intentionally created defect arrays was implemented to enhance the understanding of defect detection tools [8].

Many studies related to fault detection and process optimization in wafer fabrication have been accomplished. Especially, fault detection that influence product quality has been achieved because when defects on a wafer form spatial patterns, it is usually a clue to the identification of equipment problems or process variations. The objectives of these studies were focused on detecting faults and adjusting the operational conditions for process optimization and to produce wafers with no defects. For the detection of faults, data mining tools are needed to analyze input-output data using models or rules. In order to select a proper method from various data mining methodologies, a data mining roadmap was generated in this study to assist in the selection of an appropriate methodology. The roadmap provided the methodologies selected for the data model to predict process quality and the rule set to seek the optimal operational conditions according to the model output. After selecting the method, data acquired from the target process is used in data mining. The collected data should be sufficient in number and clean enough to perform the data mining. Due to insufficient data for wafer's quality in this research quality evaluation was performed according to sampling inspection, not total inspection. The lack of data causes an over-fitted model and incorrect rules. To overcome these problems, an appropriate data preprocessing of the bootstrap method was used to generate additional data sufficient for a total inspection. Improvement of model performance was observed from the results.

In the following, the target process of the ingot fabrication process, the proposed road map for data mining, the applied data mining techniques, and the application to the experimental data are presented.

2. WAFER FABRICATION

2.1 Wafers for semiconductors

Wafers are used in manufacturing memory or non-memory semiconductor 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. In order to enlarge the capacity of memory and non-memory chips, larger-diameter wafers and strict quality assessment are required from wafer manufacturers. To cope with these requirements, optimization of wafer fabrication is essential.

Wafer fabrication processes consist of crystal growth, wafer slicing, wafer polishing and cleaning, and epitaxial deposition. The factors of some process exist that cause defects. Nevertheless, it is difficult to return and maintain the optimal solutions for a given process conditions, because real-time analysis cannot be achieved in wafer fabrication. In this study, we develop the management system and evaluate its performance that analyzes process data related to yield and quality in wafer manufacturing and also it controls the operating parameters based on the process status.

2.2 Ingot data

Ingot is the first material manufactured in wafer fabrication. In ingot fabrication, the set-points for handling of the position or rotation of ingots and the control parameters are adjusted for quality management. These operating parameters play an important role in wafer quality and size control. Thus, proper handling of the parameters is needed for improvement of productivity and yield. The operating parameters are used as inputs in modeling. The quality parameters consist of five concentration values, and six defect values. Four of these were used for outputs in modeling for the present study. Figure 1 shows how to slice the ingot and to inspect the quality of wafers from the ingot.

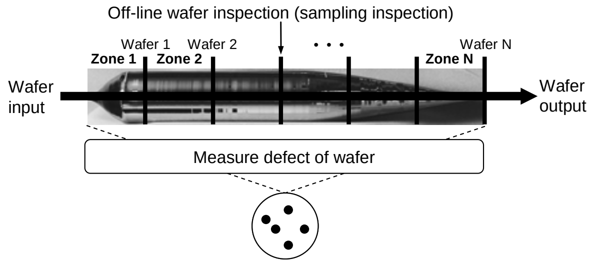

Fig. 1. Sampling inspection of ingot in measuring quality.

3. DESIGN OF DATAMINING ROADMAP

3.1 Datamining

Data mining techniques, such as extracting useful information from data or constructing an application model, are well suited to improve process performance and product quality. Data mining includes data selection, preprocessing, transformation, data mining and interpretation (Fig. 2). In order to obtain necessary information from the data, a series of the data processing methods were applied to the data obtained from the real wafer process.

In the case of the insufficient data collected, a data selection and preprocessing procedure should be considered an important stage (Fig.2). The raw data used in this study were insufficient to extract rules because the data was mainly obtained under normal process conditions. The factors that affect the final quality were initially extracted. The statistical methods such as the Monte Carlo/Bootstrap method were utilized to fill vacancies in the data and overcome data shortages.

The transformation step, as shown in Fig. 2, is one of the basic stages of data mining applications that can be applied to time-series data. This step was not used in this study as the wafer process data was not in the time-series format.

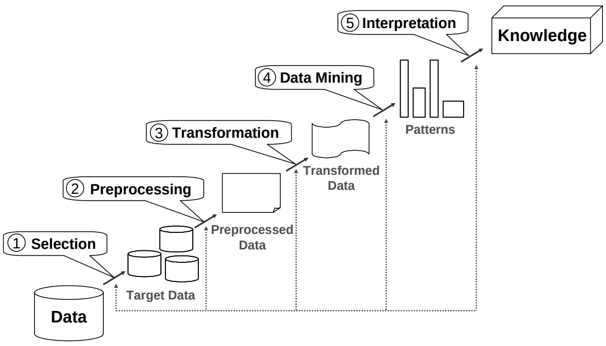

Fig. 2. Processes of data mining in knowledge creation.

3.2 Data mining roadmap

Many types of the data mining techniques can be applied to knowledge extraction. Figure 2 shows the data mining application procedure. Not all of the steps are used in data mining. Selection of the techniques depends on data features and mining targets. Therefore, selection of proper mining techniques is very important for reliable results.

In this study, we proposed the roadmap for data mining. Figure 3 shows the proposed roadmap. A selection was made with reference to the methods and procedures for diagnosis and optimization of the ingot process by referring to the roadmap. The selected methods were data generation with the bootstrap method, prediction modeling of dynamic polynomial neural network. Data generation was used for data preprocessing, prediction modeling was applied to predict the quality of wafers.

3.3 Application of datamining

3.3.1 Data preprocessing in reducing data effects

The collected data from assembly lines may be confined to specific cases; thus, the quality data are not always uniformly distributed. Insufficient data results in unreliable model prediction. It may be difficult to extract rules that encompass

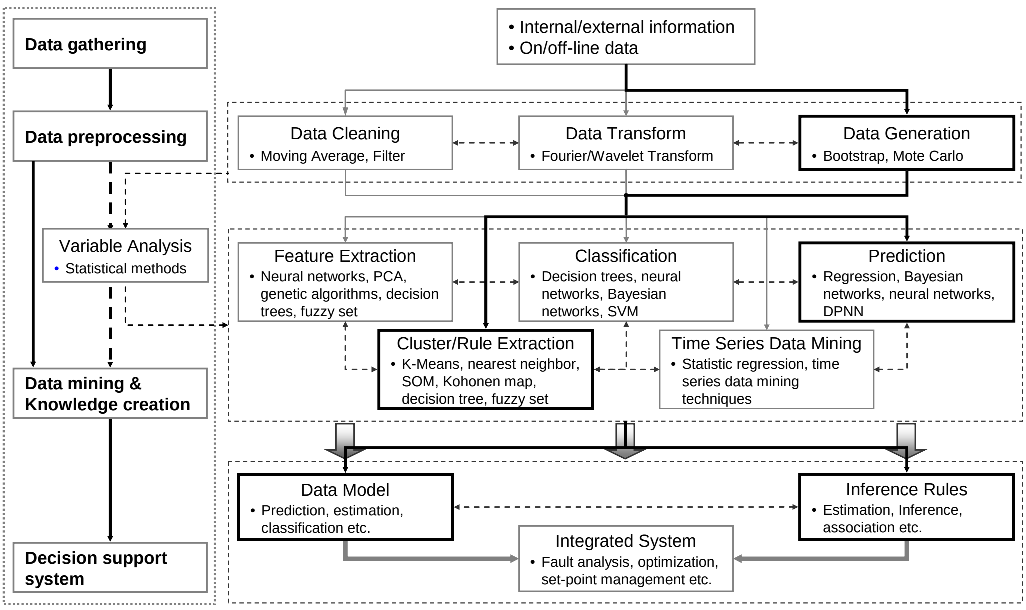

Fig. 3. Data mining roadmap proposed in this study.

the general case with limited data. Low-frequency data can be traced to error values in rule extraction. In order to solve these problems, data preprocessing is required by adding data and improving performance. In this study, the Bootstrap method, which is a type of Monte Carlo method, and multiple regression models were applied to compensate leakage data caused by sampling inspection. This stage of data generation is a part of the roadmap.

3.3.2 Data modeling in quality prediction

In prediction models, inputs can affect the performance of the models. Selection of inputs corresponding to data characteristics is necessary to improve model performance, as unnecessary inputs may influence strongly on prediction results. Therefore, the principal inputs that greatly influence model accuracy were selected. For evaluation of the function, the dynamic polynomial neural network (DPNN) was used, as it has the advantages that requires only small computation and is very useful in modeling with high-dimension variables and a large amount of data. This method can also select essential inputs through the modeling stages, so that it may be able to improve accuracy of models. This stage of prediction modeling is another part of the roadmap.

3.4 Process Management System in Ingot Fabrication

The models designed and the rules extracted are integrated into the proposed process management system. This system will play an important quality management in ingot manufacturing. The quality will be predicted by models and the control parameters will be modified by rules on-line. The final system is shown in Fig. 4.

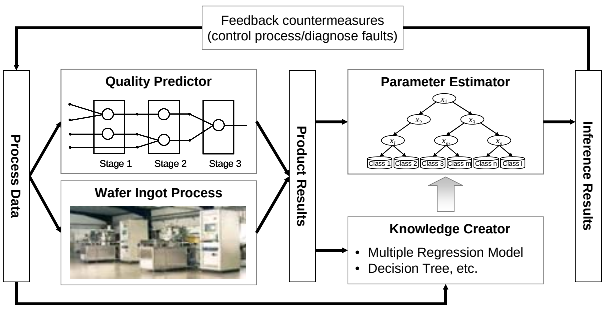

Fig 4. Structure of the proposed process management system

4. APPLICATION OF DATA MINING TOOLS

The process data have two characteristics. First, trace data for control parameters are collected by real-time measurement, but measurement data for 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. Second, quality data are included in three cases. The problem of insufficient data results in inadequate performance of the model. The Bootstrap method with data generation is then used. It is then followed by construction of the prediction model using the DPNN.

4.1 Bootstrap method

The bootstrap method was presented by Efron and Tibshirani [9]. In this study, the term bootstrap refers to Monte Carlo simulation that treats the original sample as a pseudo-population or as an estimate of the population where no parametric assumptions are made about the underlying population that generated the random sample. Instead, we use the sample as an estimate of the population.

4.2 Dynamic polynomial neural network (DPNN)

Polynomial neural network (PNN) based on GMDH algorithm is of value to model a system from many observed data and input variables. It is widely used for modeling of dynamic systems, prediction, and artificial intelligent control because of its advantages in data handling. The basic structure of PNN is two inputs and one output for each node. Figure 5 includes the recurrent inputs with one-to-n time-delayed output variables. Thus, it is called the PNN as DPNN [34-36].

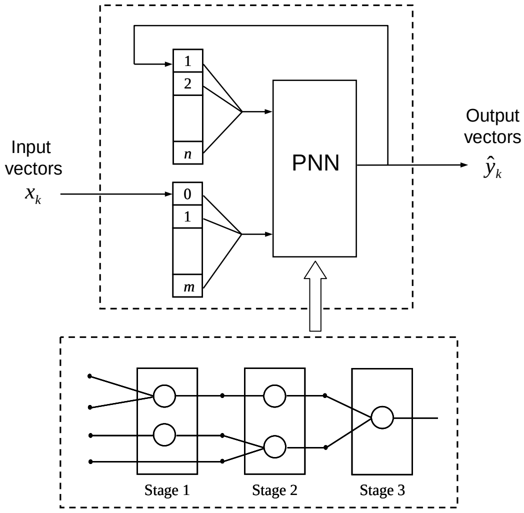

Fig. 5. Basic structure of DPNN.

5. EXPERIMENTAL RESULTS

5.1. Trace and Measurement Data of Ingots

The collected data from ingot fabrication on the factory assembly lines are shown in Fig.6. 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 online. The measurement parameter data are gathered by sampling inspection and used for quality analysis.

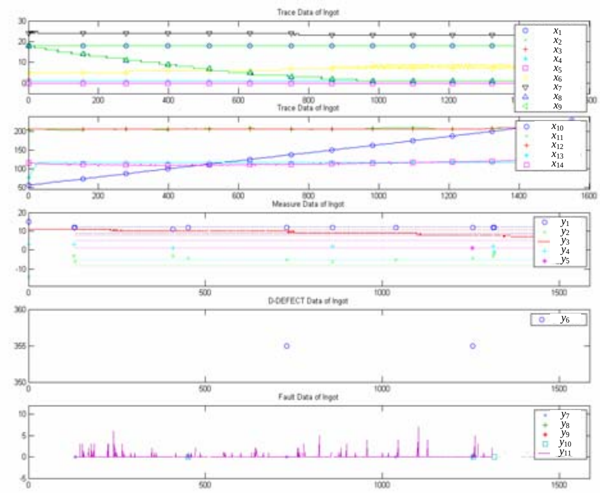

Fig. 6. Trace and measurement of parameter data.

The left column of Table 1 shows puller trace data. Forty-eight process parameters are collected by one data set per one minute from pullers. Among the parameter data, 18 important parameter data are stored in the database and used for process analysis. The position of the trace data represents the value of the wafer position (body length) of the measurement data. The second column of Table 1 shows the puller measurement data collected off-line. The data were measured by sampling inspection after slicing the ingot into wafers, and indicates the ingot growth-related parameters. The wafer position corresponds to the position of the trace data.

Table 1. Trace and measurement data of wafer.

No	Trace parameter	Measurement parameter
1	OBSERV_TIME	POSITION
2	POSITION	OXYGEN
3	SD_ROT_SET	ORG
4	SD_ROTATION	RES
5	SD_LIFT_SET	RRG
6	SD_LIFT	SPV
7	CR_LIFT	D_DEFECT
8	CR_POSITION	I_DEFECT
9	CR_ROTATE	OISF
10	CZ_DIA	SWIRL
11	CZ_DIA_SET	SLIP
12	AR_GAS_FLOW	LLPD
13	CHAMB_PRESS	
14	UP_MAG_LOAD	
15	LO_MAG_LOAD	
16	HEAT_POWER	

The trace parameter data were gathered by online measurement, as shown in Fig. 7. The problem of insufficient data exists in modeling or at the stage of rule extraction. It may be solved by merging data from several pullers. Since each puller has a unique recipe, the features of each process are different. In this study, one puller data were added with data generated at the preprocessing stage at which the number of the target data can be the same as that of the input data. Figure 7 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. 7. Data generation for quality data.

5.2 Quality Prediction and Variable Selection using DPNN

5.2.1 Data modeling using one puller data (Case 1)

Figures 8 to 11 show the test results using the trained DPNN model with unobserved data. The prediction models were designed for quality prediction corresponding to Oxygen, ORG (Oxygen Gradient), RES (Resistivity), and RRG (Resistivity Gradient). In the case of RES, the model can be designed by one puller with sufficient data. And the model performance is also adequate to predict the quality of wafers with RES. However, three other parameter data are not sufficient to design a good performance model. The model was not trained well with one puller data. Table 2 shows the training and testing results and the selected inputs from modeling using one puller data.

5.2.2 Advanced modeling based on data generation (Case 2)

The preprocessing stage was required to compensate for weak points caused by insufficient data before applying the main data mining techniques. The Bootstrap method is used to solve the data problem. The Bootstrap method can generate reasonable data to design the data models and improve the model performance. Figures 12 to 15 show the improved results augmented by data generation. Table 3 shows the prediction results and the input selection, where AR gas flow, chamber pressure and heat power were selected. These control parameters have strong influence on the wafer quality, so these have to be carefully handled in fabrication processes.

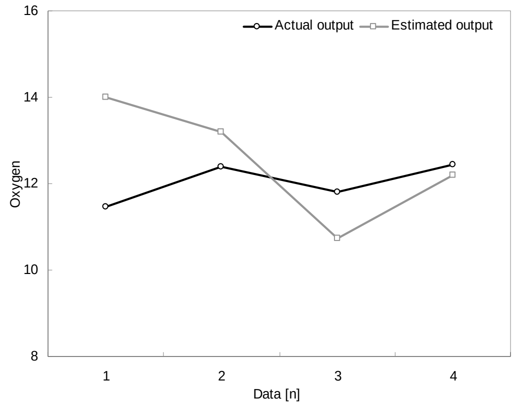

Fig. 8. Prediction for Oxygen.

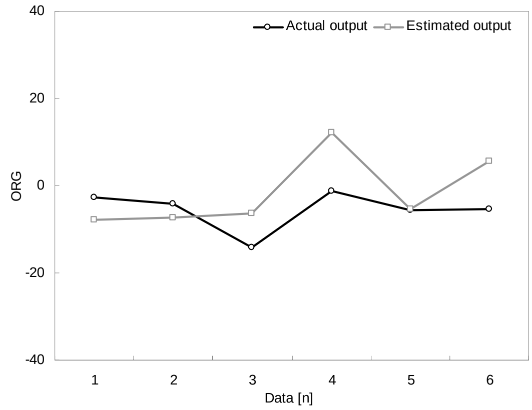

Fig. 9. Prediction for ORG.

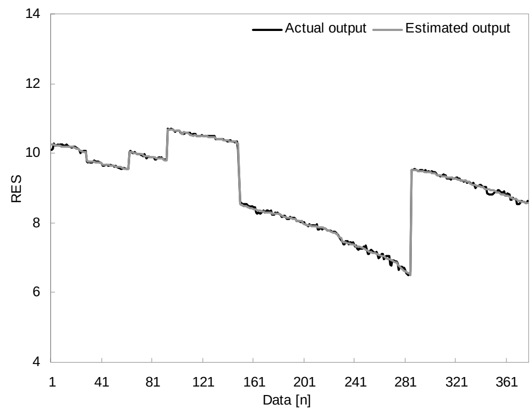

Fig. 10. Prediction for RES.

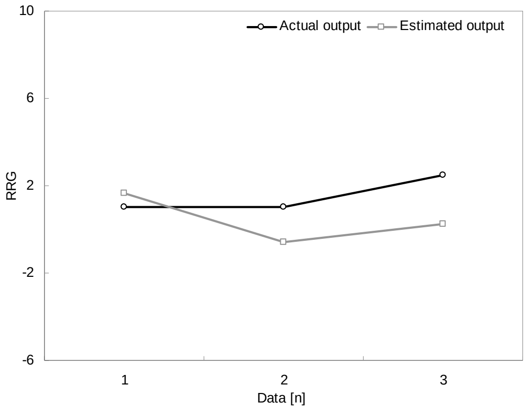

Fig. 11. Prediction for RRG.

Table 2. Results of modeling using one puller data.

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

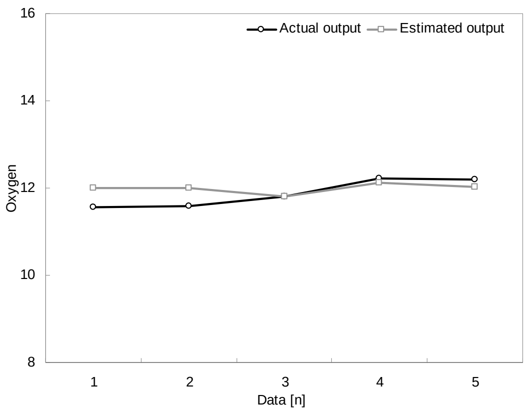

Fig. 12. Prediction for Oxygen.

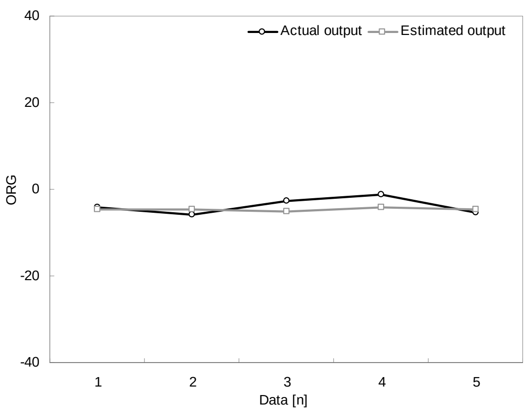

Fig. 13. Prediction for ORG.

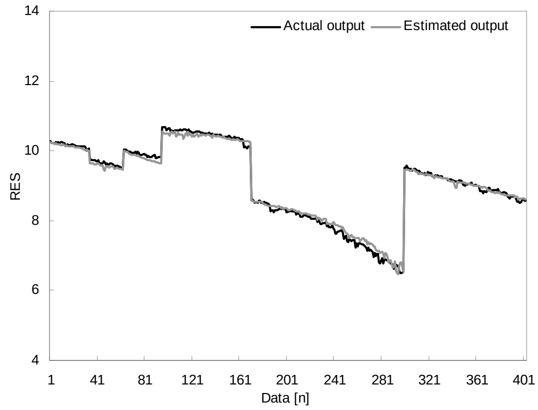

Fig. 14. Prediction for RES.

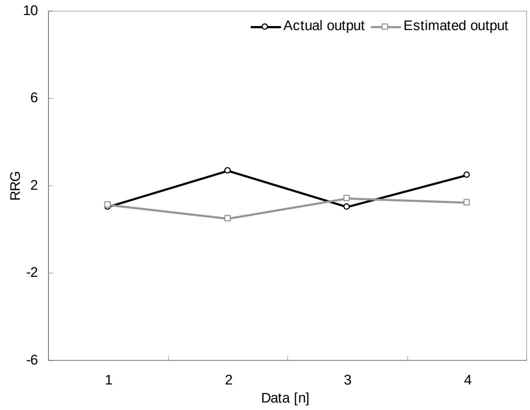

Fig. 15. Prediction for RRG.

Table 3. Modeling results with data generation.

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

5.2.3 Comparison of performance of prediction models

Table 4 shows the comparison of results for two cases of modeling. In Case 1, the models were designed for one puller with insufficient data, so that an over-fitting problem occurred. This means that a model trained by insufficient data cannot ensure the good performance of models.

In Case 2, the model trained stably by data addition using the Bootstrap method showed good performance. The results indicate that statistical data generation can reduce the effect of insufficient data. It is difficult to analyze the relationship between inputs and outputs using field data as field data are often insufficient for modeling. Thus, data pre- processing is required. In this study, an adequate descriptive model was designed by data generation.

Table 4. Comparison of results for two cases.

Value	Case	Oxygen	ORG	RES	RRG
Learning error	1	9.70e-015	4.81e-014	0.0632	4.52e-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

The ingot fabrication process is one of the important sub-processes in wafer manufacturing. 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. This function can be useful for low-defect wafer fabrication. 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 used the bootstrap method for data generation, and then designed models using the DPNN. Through the stages, the models and rules can be improved and their performance was reasonable.

One aim of this study was to design a roadmap for data mining, because it is difficult to determine which method is the best for a given target plant. Her, we proposed a roadmap, based on which the applied methods were selected. The models will be utilized to integrate both the diagnosis and the optimization systems of the ingot fabrication process.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Commerce, Industrial and Energy, IMS International Program.

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