Development of a virtual metrology for high-mix TFT-LCD manufacturing processes*

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Abstract: Nowadays, TFT-LCD manufacturing has become a very complex process, in which many different products being manufactured with many different tools. The ability to predict the quality of product in such a high-mix system is critical to developing and maintaining a high yield. In this paper, a statistical method is proposed for building a virtual metrology model from a number of products using a high-mix manufacturing process. Stepwise regression is used to select "key variables" that really affect the quality of the products. Multivariate analysis of covariance is also proposed for simultaneously applying the selected variables and product effect. This framework provides a systematic method of building a processing quality prediction system for a high-mix manufacturing process. The experimental results show that the proposed quality prognostic system can not only estimate the critical dimension accurately but also detect potentially faulty glasses.

Key words: stepwise regression; virtual metrology; MANCOVA; thin film transistor liquid crystal display
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1. Introduction

In recent years, the thin-film transistor-liquid crystal display (TFT-LCD) has become more and more important in optical electrical industry across the world. Many devices, such as computers, notebooks, digital cameras and flat panel TVs, need TFTL-LCDs to display the information content. With the extensive application of TFT-LCDs, more and more manufacturers are participating in the high-tech industry, thereby making profits smaller and smaller. Therefore, improving the yield for the manufacturing process has been viewed as an important competitiveness determinant for TFT-LCD manufacturers. In general, a TFT-LCD manufacturing process consists of three main sub-processes: array, cell and module processes. The final quality of products in the array process is one of the most critical steps[1]. Similar to semiconductor wafer fabrication, the glass of the array process must be processed 5–7 times through cleaning, coating, exposure, developing, etching and strip. In each step, the equality of the processed glass has a serious impact on the final product yield. So, it is important to monitor the glass-state data, such as critical dimension, uniformity and thickness, and to find faulty glasses in the shortest possible time during each processed step. However, most of glass-states lack an *in situ* sensor to provide real time information in each processed step, and usually they are measured offline and less frequently than every glass, which can lead to a number of glasses being scrapped before a fault is detected[2]. To remedy this problem, most of the TFT-LCD manufacturers exert much effort to implement and improve highly automated and precisely monitored facilities throughout the complex manufacturing process[3]. Nonetheless, process variations still exist and are reflected in real-time measurements of process variables, such as temperature, pressure, power and flow rate. These real time measurements provide valuable information about the tool status and may be directly correlated with the final quality of the glass. Engineers attend to the investigation of these process variables in order to enhance the yield rate. A better approach is to apply virtual metrology (VM) technology, which can predict the process quality of every glass with the process data of production equipment. Then, the objective of real-time glass-to-glass quality monitoring without interrupting the normal operations can be achieved.

Previous literature is quite rich in different VM schemes as well as various design approaches for each scheme. Generally, these methods can be divided into two groups: nonlinear methods[4, 5] and linear methods[6, 7]. Although these methods have been proven to be useful in batch manufacturing, they neglect the inherent characteristics of the process. In the modern and TFT-LCD manufacturing industry, production resembles an automated assembly line in which many similar products with different specifications are manufactured by the same tool. In this high-mix manufacturing process, the VM developed for a single product cannot be directly used. In order to overcome this problem, a new processing quality prediction system has been developed for sophisticated high-mix manufacturing processes. Using stepwise regression, key variables with physical meaning are selected to build a VM model, and the collinearities and high dimensions of the process data can also be reduced. Another contribution is that a multivariate analysis of covariance (MANCOVA) method is cast into the VM framework. Using this VM algorithm, the quality of products with different specifications can be predicted during manufacture. This can not only enhance (or even replace) direct metrology

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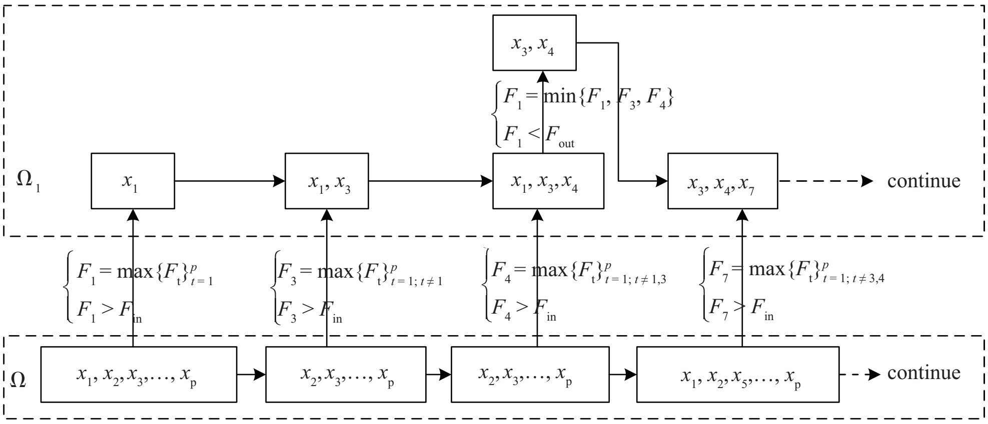

Fig. 1. Flowchart of stepwise regression.

operations but also increase manufacturing efficiency.

2. Systematic approach for the development of VM

Consider numerous products of the same recipe, which are labeled by an index $i = 1, 2, \cdots, n$ according to their sequence of the finishing quality measured step. These products contain J specifications. Here, n sets of historical data are assumed to be collected, including process data (X_i, $i = 1, 2, \cdots, n$) and the corresponding actual measurement values ($y_i, i = 1, 2, \cdots, n$), where each set of process data contains p sensor variables (SVs) , namely $X_i = \left[x_{i,1}, x_{i,2}, \cdots, x_{i,p}\right]^T$. These highly dimensional parameters may be collinear.

In general, a number of steps, including data collection and filtering, variables and model structure selection, model identification and model validation, are essential for the development of a successful VM. Each step is crucial. A number of studies have focused on data collection and preprocessing, and topics such as data compression, data missing and outlier detection are discussed [8, 9]. This paper focuses on variables selection, model identification and validation based on a statistical method.

2.1. Key variable selection based on a statistical method

As mentioned above, these p SVs in $\Omega = \left\{x_1, x_2, \cdots, x_p\right\}$ may be highly dimensional and collinear. Selecting the correct subset is challenging yet critical in developing useful VM models. In the literature, many compression algorithms, such as principal component analysis (PCA) and partial least square (PLS), have been described. These methods can deal with high dimensionality and collinearities in data by projecting the original process variables onto a space defined by the orthogonal principal components (PC) or latent variables (LV). However, the field engineer may not understand the physical meaning of PC/LV. Thus, a variable selection method is used in this paper. With the aim of finding some "key variables" $\Omega_1 = \{x_1, x_2, \cdots, x_k\}$ $(k < p)$ that affect the quality of products in the manufacturing process. Then, the selected parameters are used to fit the multiple regression model,

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \varepsilon, \tag{1}$$

where ε is the estimated error.

Stepwise regression is widely used for variable selection in a linear system. The procedure iteratively constructs a sequence of regression models by adding or removing variables at each step. The criterion for adding or removing a variable at any step is usually expressed in terms of a partial F_t. Let F_{in} be the value of the F-random variable for adding a variable to the model, and let F_{out} be the value of the F-random variable for removing a variable from the model. The requirement of $F_{in} > F_{out}$ ensures that inserting a variable is more difficult than removing one. A complete description of the algorithm is as follow[10].

Step 1: Determine the thresholds of the probability of a type I error (e.g., $\alpha_{in} = 0.05, \alpha_{out} = 0.1$) and the corresponding confidence level in partial F-statistic(F_{in} and F_{out}).

Step 2: Assume set $\Omega_1 = \{x_1, x_2, \cdots, x_k\}$, which is a subset of $\Omega = \left\{x_1, x_2, \cdots, x_p\right\}$, is selected by the model (1). Now the remaining $p - k$ candidate variables are examined one by one and its corresponding partial F-statistic $\{F_t\}_{t=1}^{p-k}$ can be calculated.

Step 3: If $\left(F_q = \max\{F_t\}_{t=1}^{p-k}\right) > F_{in}$, then add x_q to the subset Ω_1, or else go to Step 4.

Step 4: $k + 1$ tested models are constructed with all variables in $\Omega_1 = \{x_1, x_2, \cdots, x_k, x_{k+1}\}$ except x_i $(i = 1, 2, \cdots, k + 1)$ in turn. The corresponding partial F-statistic $\{F_t\}_{t=1}^{k+1}$ is calculated.

Step 5: If $\left(F_q = \min\{F_t\}_{t=1}^{k+1}\right) < F_{out}$, then hold the subset Ω_1, or else remove x_q from the subset Ω_1.

Step 6: Repeat steps 2 to 5 until no other variables can be added to or removed from the model.

The details of stepwise regression are shown in Fig.1. In the adding step, the variable with maximal partial F_t and larger than F_{in} should be selected from Ω. In the elimination step, the variable with minimal partial F_t and less than F_{out} should be removing from Ω_1. For both steps, the F_t is calculated as

$$F_t = \frac{SS_R\left(x_t, x_1, x_2, ..., x_k\right) - SS_R\left(x_1, x_2, ..., x_k\right)}{MS_E\left(x_t, x_1, x_2, ..., x_k\right)}, \tag{2}$$

where $SS_R(\cdot)$ is the residual sum of squares due to regression, and $MS_E\left(x_t, x_1, x_2, ..., x_k\right)$ denotes the mean square error for the model containing both x_t and $x_1, x_2, ..., x_k$.

Finally, the variables selected for the VM model are termed "key variables", which directly affect the quality of products and may contain important information regarding the source of variation of the current process condition.

2.2. VM development based on MANCOVA

As mentioned above, there are J types of product specification. Based on model (1), the product effect should be considered in the VM model. Then, the model can be constructed by MANCOVA [11],

$$\hat{y}_{i,j} = \mu + \tau_j + B^T X_i + \varepsilon, \tag{3}$$

where $\hat{y}_{i,j}$ is the i^{th} product with j^{th} specification, μ is the mean of all products (y_i), τ_j is the product effect of the j^{th} specification, $\sum_{j=1}^{J}\tau_j = 0$; $X_i = \left[1, x_{i,1}, x_{i,2}, \cdots, x_{i,k}\right]^T$ denotes the key variables selected by stepwise regression, $B = [\beta_0, \beta_1, \beta_2, \cdots, \beta_k]^T$ is a regression coefficient and ε is the estimated error.

The matrix form of Eq. (3) is

$$Y = \begin{bmatrix} 1 & \underbrace{\begin{matrix}\delta_{1,1} & \dots & \delta_{1,J} \\ \delta_{2,1} & \dots & \delta_{2,J} \\ \vdots & \cdots & \vdots \\ \delta_{n,1} & \cdots & \delta_{n,J}\end{matrix}}_{J} & \underbrace{\begin{matrix} x_{1,1} & \dots & x_{1,k} \\ x_{2,1} & \dots & x_{2,k} \\ \vdots & \cdots & \vdots \\ x_{n,1} & \cdots & x_{n,k}\end{matrix}}_{k} \end{bmatrix} \begin{bmatrix} \mu \\ \tau_1 \\ \vdots \\ \tau_J \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \tag{4}$$

where $\delta_{i,j} \in \left\{ \delta_{i,j} \in \{0,1\} \,\middle|\, \sum_{j=1}^{J} \delta_{i,j} = 1,\ i = 1, \cdots, n \right\}$. As shown in Eq. (4), The regression B and product effects τ_j can be calculated via an ordinary least squares algorithm.

2.3. Evaluation of VM

To evaluate how well a VM model fits the relationship between the input data and the metrology target values, the root mean square error of prediction and the mean absolute percentage error are used,

$$\text{RMSE} = \frac{1}{n}\sqrt{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}, \tag{5}$$

$$\text{MAPE} = \frac{1}{n}\sum_{i=1}^{n}\frac{|\hat{y}_i - y_i|}{y_i} \times 100\%, \tag{6}$$

where y_i and $\hat{y}_i$ are the actual target and predicted value of the i^{th} test wafer, respectively.

3. Experimental results

This section describes an investigation into a wet etching process for the fabrication of TFT-LCDs deposited with low resistance data lines of Mo/Al/Mo, as shown in Fig. 2. In TFT-LCD manufacturing, the wet chemical etch proceeds with spraying the glass substrate with the etchant solution. The glass substrate is swung from side to side by the servo mechanism. This mechanical agitation is required to ensure etch uniformity and a consistent etch rate. Then, chemical reactions occur at the surface and the products from the surface are removed by diffusion.

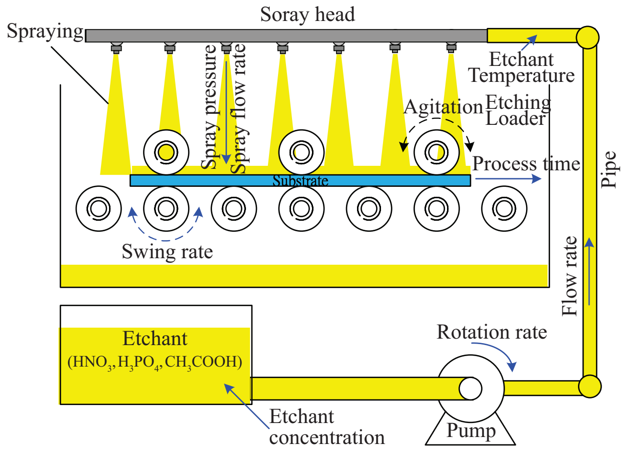

Fig. 2. Schematic diagram of the wet etching process.

With this type of process, the CD is known to be affected by several factors, such as the etching time, the temperature of the etchant solution, the spraying pressure, the flow rate of the etchant and the chemical consumption. The sensor data were collected from the etching process of a TFT-LCD manufacturing plant of AU Optronics Corporation local in Taiwan. The example involves 20 sensor data (process data; $x_{i,j}$, $j = 1, 2, \cdots, 20$) collected from July to December 2009. The sample number of the process data is 34096, involving seven specifications (the 24-inch has four specifications, the 32-inch has two specifications and the 42-inch has one specification; see Fig. 2). However, not all of their corresponding actual CDs (y_i) were measured, because only 1–2 glasses of a cassette were selected as sample glasses, whose CD value were measured to monitor the quality of the whole cassette. Consequently, these 671 glasses of process data and their corresponding actual metrology values can be used as data to build a model of the wet etching process. Among the 671 glasses, the first 274 glasses were used to obtain data with which to establish the model, and the remaining 397 glasses were used to validate the model.

In this etching process, not all process data are critical affect the CD. To reduce the dimension of modeling, statistical stepwise regression was used for input variable selection. As a result of stepwise regression, the temperature of the etchant solution ($x_{i,1}$), the flow rate of the etchant ($x_{i,2}$) and the chemical consumption ($x_{i,3}$) were chosen as inputs to the Multiple Linear Regression. According to the physical properties of the etching process and the experience of the equipment engineers, the corresponding coefficients must be less than zero. Thus, the parameters can be calculated by solving the following optimal objective function with constraints,

$$\begin{aligned} &\min J = \left(y_{i,j} - \sum_{t=1}^{3}\beta_t x_{i,t} - \beta_0 - \mu - \tau_j\right)^2 \\ &s.t.\ \beta_t < 0, \quad t = 1, 2, 3, \\ &\quad \sum_{j=1}^{7}\tau_j = 0, \\ &\quad \mu = \frac{1}{274}\sum_{i=1}^{274} y_i. \end{aligned} \tag{7}$$

Then, the VM model is obtained,

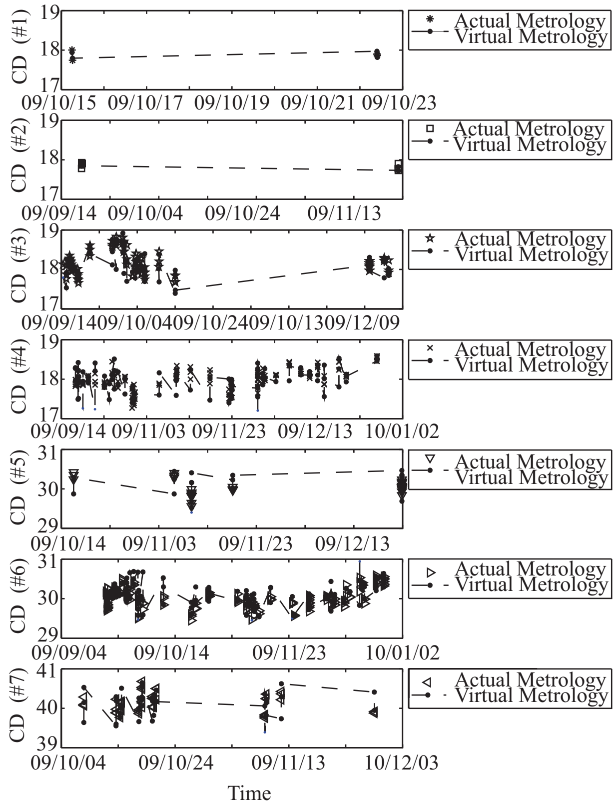

Fig. 3. Performance with VM for high-mix products.

$$\hat{y}_{i,j} = \beta_1 x_{i,1} + \beta_2 x_{i,2} + \beta_3 x_{i,3} + \beta_0 + \mu + \tau_j. \quad (8)$$

The training result of VM was as follows: RMSE = 0.2148 and MAPE = 0.73%. To test the performance, the CDs of the remaining 397 glasses with seven specifications were predicted by the developed VM model. Figure. 3 shows the conjecture results. The RMSE and MAPE are 0.2515 and 0.81%, respectively. To further illustrate the capability of the proposed VM, a product #3 processed in one day was taken, for example. As shown in Fig. 4, the RMSE and MAPE are 0.2438 and 0.97%. Also, the maximum predicted error is 0.4980 and emerged in number 6. It can be seen that the VM predictor is accurate enough to be implemented in an actual TFT-LCD manufacturing process.

Our VM model aims not only to predict metrology values but also to monitor the glass-to-glass quality, values of which are outside the control limits. Taking product #5, for example, 1445 glasses were processed in November 2009. Figure 5 shows the predicted values for product #5. In this specification, the upper control limits (UCL) and the lower control limits (LCL) are 29.5 and 30.5, respectively. Using the proposed VM, four out of five abnormal products were detected while one abnormal glass was misclassified. So, the accurate ratio of prediction was 80%. Although our VM model missed one glass, the highly suspect glasses whose actual target values were very far from the control limit (four glasses) were detected as well. In terms of the workload of measurement for 1445 glasses, the detection time was reduced greatly. On the other hand, four scrapped glasses were removed in this etching process and the follow-up production costs were also saved.

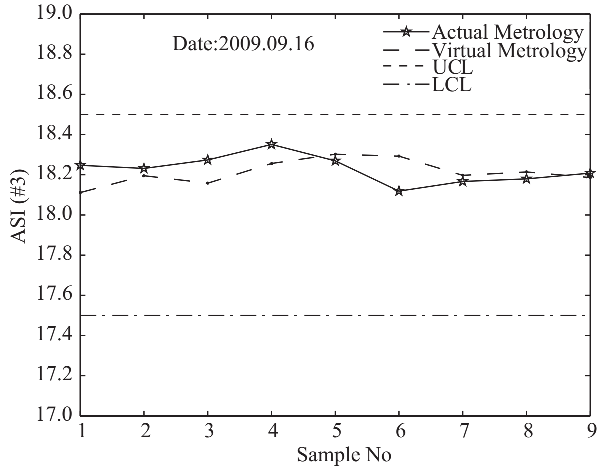

Fig. 4. Performance with VM for product #3 in one day.

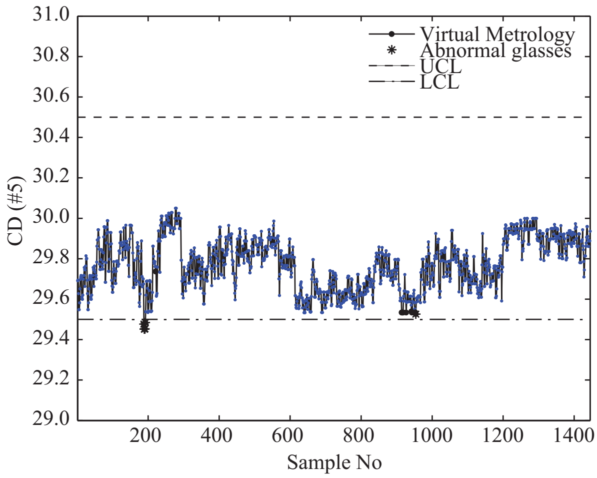

Fig. 5. Monitoring process for product #5 using the proposed VM.

4. Conclusion

In this paper, we describe the development of a VM model based on statistical methods and modern data-mining techniques. The process data can be selected directly as key variables by a stepwise linear regression method. The experimental results show that the number of input variables decreased significantly. Taking the product effects into consideration, a high-mix VM model was presented using MANCOVA. Based on the conjecture/prediction results of the illustrative example, this quality prognostic scheme is believed to be feasible and able to conjecture/predict product quality efficiently and effectively.

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