# Multivariate Classification of BPSG Thin Films Using Mahalanobis Distances

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## Abstract

Infrared absorption spectra of borophosphosilicate glass (BPSG) thin films were collected
to develop a rapid classification method for determining if the films are within the desired specifi-
cations. Classification of samples into good and bad categories was performed using principal
component analysis applied to the spectra. Mahalanobis distances were used as the classification
metric. The highest overall percentage of correct classification of samples based upon their spec-
tra was 91.6%.

## Introduction

In the microelectronics industry, the establishment and maintenance of multivariate-based
spectral process monitors can be a time-consuming and expensive project. A large number of
wafers must be prepared and sacrificed in order to set up the multivariate spectral calibration
model or to change the model when the product target value changes. Normally, the calibration
of the monitor requires a large number of reference measurements to be taken off-line. In order
to save time and expense, a "reference-free" model is desired that can be built rapidly and nonde-
structively from the flow of "good material" against which process deviations could be detected.

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Fourier transform infrared (FTIR) spectroscopy is a rapid and nondestructive measurement technique that has been shown to be able to quantify all the attributes of the thin films in a single spectrum.[1-3] Mark [4] and Shah and Gemperline[5] have reported the qualitative identification of raw materials by near infrared (NIR) spectroscopy using a Mahalanobis distance classification technique. In this paper, we report the use of principal component analysis (PCA) coupled with the Mahalanobis distance metric to classify BPSG films as "good" or "bad" depending on whether or not the film properties are within a specified range of the target values for those properties.

## Experimental

The 108 BPSG thin films on 150 mm diameter silicon wafers used in this study were prepared at Intel Corporation (Santa Clara, CA) in an ASM/PTL low pressure chemical vapor deposition (LPCVD) batch reactor. The target values of these thin films are 2.1 wt% B, 6.7 wt% P, and 1.0 μm film thickness. The contents of B and P and the film thickness for all samples were measured by separate reference methods. Samples were defined as good if they were within ±5% of the target values for B and P and within ±8% of the film thickness target value. FTIR absorption spectra of the thin films were collected at the center of the wafers with an ECO-8 FTIR spectrophotometer. Various pretreatment procedures were applied to the spectra and the resulting data were analyzed using multivariate calibration and classification software written in our laboratory [6,7]. Using the reference values of B, P, and thickness, twenty-five typical "good" samples from the 108 thin films were used to build the classification model. The rest of the samples were tested as unknown samples. The PCA and normalized Mahalanobis distance calcula-

tions were then carried out. An unknown spectrum was classified as a "good" sample if the normalized Mahalanobis distance was less than unity.

## Results and Discussion

Three parameters of merit were used to evaluate the validity of the classification technique including accuracies of separately classifying "good" samples, "bad" samples, and all samples. According to the reference values and the desired specifications, there were 34 "good" samples and 49 "bad" samples in the test set. A sample was determined to be "bad" if any of the three parameters was out of specification. Accuracies were reported as the percentages of correctly classified samples in each of the above categories. The average number of principal components giving optimal predicted error sum of squares (PRESS) was selected to calculate the Mahalanobis distances. Preprocessing of the spectral data was performed using nine different preprocessing methods. From Figure 1, we can see that the absorbance spectra vary as the thin films' compositions and thickness vary and this variation can be related to the quality of the thin films. The preprocessing methods and their classification results were listed in Table I. Independent of preprocessing methods, the accuracy of "good" samples are all over 90% because most of the "good" samples are very similar to the samples in the training set and only a few of them are at the boundary. Most of "bad" samples are close to the boundary of the "good" sample classification since most of these "bad" samples are only slightly outside the specifications. Therefore, it is expected that a lower accuracy would be achieved for those "bad" samples near the boundary. The highest accuracy classification was obtained using a pathlength correction that scaled the spectral intensity by the relative measured film thickness. Most of the misclassified "bad" samples came

from the samples with film thickness within the specification and B content outside the specification range. This implies that the classification model is dominated by film thickness variation. Pathlength correction methods that remove the effects of film thickness result in the highest accuracy.

## Conclusions

PCA coupled with a Mahalanobis distance metric applied to FTIR absorbance spectral data has been demonstrated to be capable of differentiating "bad" thin films from "good" films. The classification is dominated by the quality of film thickness. By removing the effect of film thickness, better results have been achieved. Although the classification model developed in this work used B, P, and thickness reference values to define samples as "good" or "bad", the requirement for obtaining these reference values could be eliminated simply by monitoring whether a given sample yielded "good" or "bad" final product. Thus, the method presented here could be performed rapidly and inexpensively without the need for reference values. Pathlength scaling could be readily implemented since automated pathlength measurements can be performed rapidly with an ellipsometer or optical methods based upon interference fringes.

## References

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| Pretreatment Type | No. of PCs | % Correct "Good" | % Correct "Bad" | % Correct Overall |
|---|---|---|---|---|
| (1)  None | 3 | 91.2 | 83.7 | 86.7 |
| (2)  Smoothing | 3 | 91.2 | 83.7 | 86.7 |
| (4)  Pathlength Correction | 4 | 94.1 | 89.8 | 91.6 |
| (5)  First Devivative | 3 | 97.1 | 77.6 | 85.5 |
| (6)  Second Derivative | 5 | 97.1 | 46.9 | 67.5 |
| (7)  Autoscaling | 3 | 97.1 | 77.6 | 85.5 |
| (8)  Range Scaling | 3 | 97.1 | 77.6 | 85.5 |
| (9)  Variance Scaling | 3 | 97.1 | 77.6 | 85.5 |
| (10)  Normalized to Mean-centered Variance | 3 | 91.2 | 83.7 | 86.7 |
| (11)  Normalized to Unit Length | 3 | 91.2 | 83.7 | 86.7 |

**FREQUENCY (cm⁻¹)**

**ABSORBANCE**