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FT-IR Measurement of PSG and BPSG Films: An Overview

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Key Words

- BPSG
- Dielectric Films
- ECO
- FT-IR
- K-matrix
- PLS
- PSG
- Semiconductor Metrology

Introduction

The move from LSI to VLSI devices has placed more critical requirements on semiconductor process conditions. Narrow line widths and accompanying reduction in the size of all device topographic features make uniformity and reduced process temperatures important. In interlayer dielectric films, the use of boron and phosphorus dopants in silicate glass has become prevalent. The addition of these dopants lowers the temperature required to soften, or flow, the glass layer, minimizing diffusion during reflow.

Historically, phosphosilicate glass (PSG) was used to lower the reflow temperature to 1000 degrees. Borophosphosilicate glass (BPSG) lowers the temperature required to soften the glass layer an additional 100 degrees. An optimal application of the chemical vapor deposition (CVD) glass assures higher device yield.

The optimization of reactor performance and the need for routine film evaluation make a quick determination of these dopant levels desirable. Though several methods have been utilized, the advantage of Fourier Transform Infrared (FT-IR) measurements is that boron, phosphorus and glass thickness can be simultaneously determined in a relatively fast (one minute), non-contact procedure.

The desirability of measuring BPSG films by FT-IR has been recognized for some time; however, the advent of both FT-IR systems designed to handle wafers and the incorporation of sophisticated computer methods of analysis have made the technique more applicable.

Two methods of analysis, K-matrix and partial least squares (PLS), are available on Thermo Scientific metrology systems. The more classical approach to quantitative infrared (IR) analysis is called the K-matrix method. It involves the assignment of bands in the infrared spectrum known to be characteristic of various types of chemical bonds (for example, the Si-0 bond of a glass film). This method is popular because it is the first method applied to the analysis and because the calibration of the method requires relatively few standards. It has been applied successfully to the measurement of phosphorus in PSG, boron in BPSG, and occasionally, though with much more difficulty, to phosphorus in BPSG. The K-matrix method is more successful with atmospheric pressure chemical vapor deposition (APCVD) films for determining phosphorus concentration than with low pressure chemical vapor deposition (LPCVD) or plasma enhanced chemical vapor deposition (PECVD) films. Annealing of BPSG wafers, particularly from LPCVD and PECVD systems, makes the likelihood of successful phosphorus determination much higher.

Three distinct areas must typically be defined in the IR spectrum, one each for boron, phosphorus and glass thickness, if it is to be measured by IR. A minimum of four calibration samples is required for the proper analysis; ideally at least six samples with randomly varying amounts of boron and phosphorus and glass thickness are used.

Using band treatment, the baseline adjustment technique and calibration, the K-matrix technique can predict boron concentrations to within 0.3 to 0.5 wt. %, depending upon how narrow a concentration range is to be monitored and how representative the calibration samples are of the final analysis wafers. Phosphorus concentrations in PSG films can occasionally be predicted as closely, but in BPSG, concentrations usually do not approach the 0.5 wt. % level and more commonly are at 0.7 wt. % or worse. Glass film thickness can also be determined and found typically to be within a few hundred angstroms by this method.

The second method of analysis, PLS, is a statistical modeling approach to quantitative analysis well suited to analyzing BPSG because it deals better with the band overlaps and component interactions common in these types of films. The PLS method accurately predicts the concentration of unknown samples, but requires more references to develop the method. This is because the software creates a mathematical model for the calibration and does not use required input of band location or reduction parameters. Typically, 11 calibration sample concentrations, with duplicates of each concentration pair, are recommended for proper calibration of the method.

When properly calibrated, the PLS program can predict phosphorus concentrations at 0.15 – 0.20 wt. %, boron at 0.05 – 0.15 wt. % and glass thickness at 50 to 100 Å (errors of prediction). Consistent wafer dopant levels, backside treatments and glass thickness minimize the error range and improve results.

Results and Discussion

Both the K-matrix and the PLS programs are fully integrated into the Thermo Scientific Nicolet™ ECO™ system software. The programs can be used for both single wafers and multiple wafers loaded from cassettes, and can be readily applied to multiple point analysis on the surface of the wafer. Either the SEMI star patterns or custom design sets of up to 100 coordinated pairs may be measured and referenced to the flat location or the notch.

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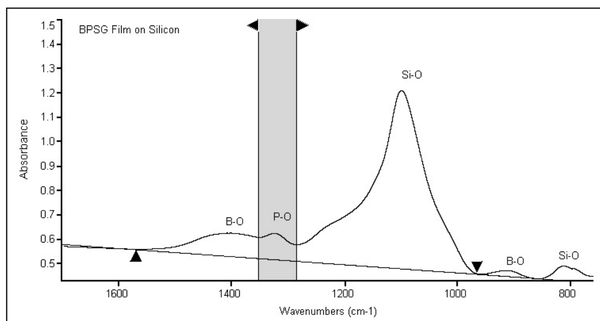

Figure 1: Infrared spectrum of a typical BPSG spectrum, showing the areas traditionally associated with boron, phosphorus and glass thickness

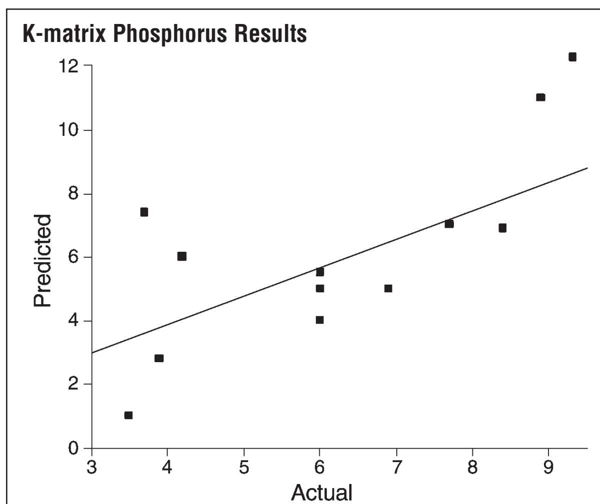

Figure 2: Plot showing the predictive ability for phosphorus using the K-matrix procedure

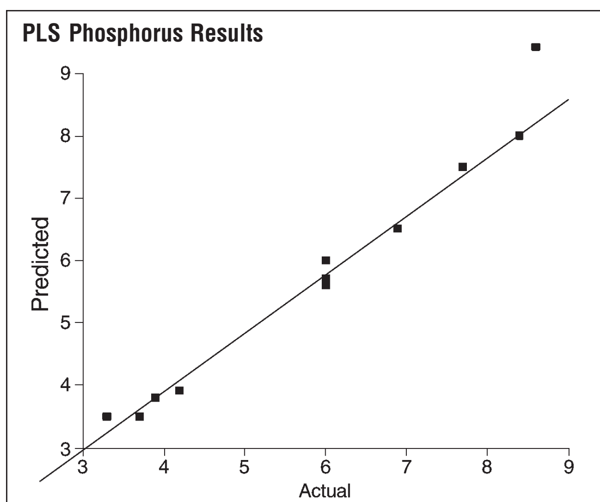

Figure 3: Plot showing the predictive ability for phosphorus using the PLS method

An example BPSG spectrum is presented in Figure 1 with the classic K-matrix band assignments one might use for that analysis. Table 1 presents a summary data set from a BPSG sample analysis comparing the capabilities of the two methods to predict concentrations. Figures 2 and 3 show the predictive ability of both K-matrix and PLS for the measurement of phosphorus. For phosphorus analysis in BPSG films, the PLS technique has significant advantages.

Table 1: Data showing the typical predictive ability for BPSG films by both the K-matrix and PLS techniques

METHOD AVERAGE PREDICTION ERROR

	Thickness	Boron	Phosphorus
K-matrix	290 Å	0.4 wt. %	1.3 wt. %
PLS	41 Å	<0.1 wt. %	0.17 wt. %

(Typical data from an analysis of densified BPSG wafers by both software methods)

Additional information on both techniques can be found in these Thermo Scientific *Application Notes*: “FT-IR Measurement of PSG and BPSG Films,” Parts I1 and II2. Part I deals with the theory of the measurement, Beer’s Law and the K-matrix analysis. Part II describes more fully our implementation of the PLS statistical method with emphasis on BPSG analysis.

Conclusion

The selection of the correct Quantitative Algorithm can greatly enhance the reliability of the results obtained.

Footnotes

1. AN50637 FT-IR Measurement of PSG and BPSG Films, *Part I: IR Principles and K-matrix Approach.*
2. AN50638 FT-IR Measurement of PSG and BPSG Films, *Part II: Partial Least Squares Approach.*

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