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## Chemometric Analysis of IR External Reflection Spectra for Quantitative Determination of BPSG Thin Films\*

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### Abstract

Infrared (IR) reflection spectroscopy has been shown to be useful for making rapid and nondestructive quantitative determinations of B and P contents and film thickness for borophosphosilicate glass (BPSG) thin films on silicon monitor wafers. Preliminary data also show that similarly precise determinations can be made for BPSG films on device wafers.

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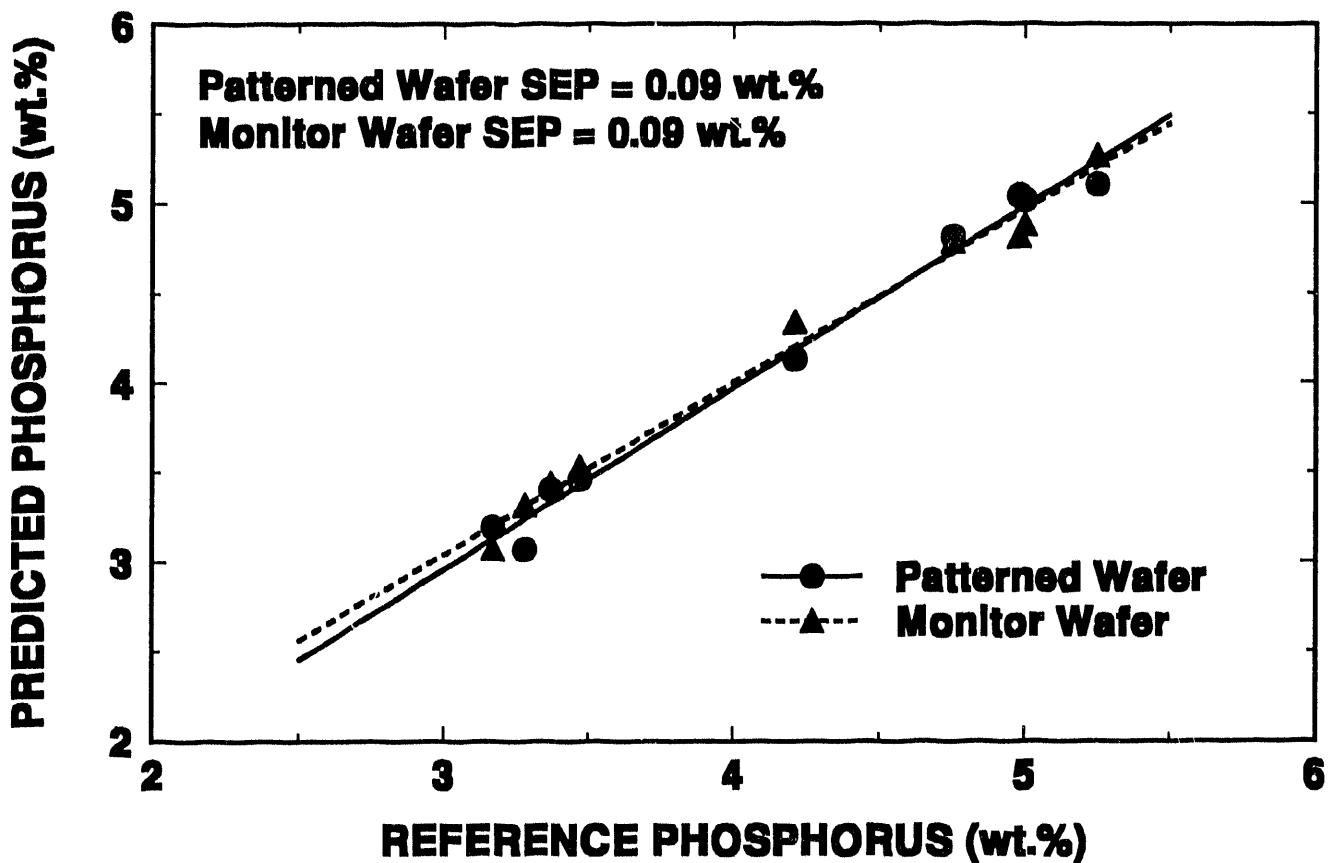
## Introduction

In prior studies, we have demonstrated IR transmission spectral data coupled with chemometric analysis could be used for precise, rapid, and nondestructive determinations of BPSG film properties. IR transmission requires that the substrate be transparent, thus monitor wafers must be used. IR reflection spectroscopy does not require the IR beam to pass through the sample, hence it offers the potential for monitoring thin-film properties when the films are deposited on patterned device wafers.

## Results and Discussion

Three BPSG thin-film calibration sets were analyzed using IR external reflection spectroscopy: (1) 21 films on undoped silicon wafers, (2) 21 films deposited on undoped silicon wafers coated with a 1000 Å thermal oxide film, and (3) 9 films deposited on actual product wafers. Chemometric analyses using partial least squares (PLS) multivariate calibration methods were performed on each spectral data set using a number of preprocessing options to optimize the calibrations. The results for the two larger BPSG calibration sets demonstrate IR reflection spectroscopy can be used to simultaneously determine B content, P content, and film thickness to precisions of 0.1 wt. %, 0.1 wt. % and 50 Å, respectively. The precisions of the determinations of B content, P content, and thickness of the films deposited on the product wafers are 0.13 wt. %, 0.09 wt. %, and 75 Å respectively. We believe the slight decrease in precision of these determinations to be due to the small number of samples in the calibration, rather than the

structure underlying the films. This has been confirmed by performing the calibrations on the corresponding set of Si monitor wafers consisting of the 9 monitor wafers deposited with BPSG under the same conditions as the device wafers. Figure 1 demonstrates the cross-validated PLS calibration results for both set of wafers for phosphorus determinations. These results demonstrate the utility of IR reflection spectroscopy coupled with chemometric data analysis as a rapid, nondestructive, and precise at-line monitor for BPSG films on actual patterned device wafers.



**Figure 1.** Comparison of the prediction abilities for phosphorus in BPSG films using PLS calibrations on patterned and monitor Si wafers.

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